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**Supplemental Mathematical Formulations:
Atmospheric Pathway**

**The Multimedia Environmental Pollutant
Assessment System (MEPAS)TM**

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March 1996

Prepared for the U.S. Department of Energy
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Pacific Northwest National Laboratory
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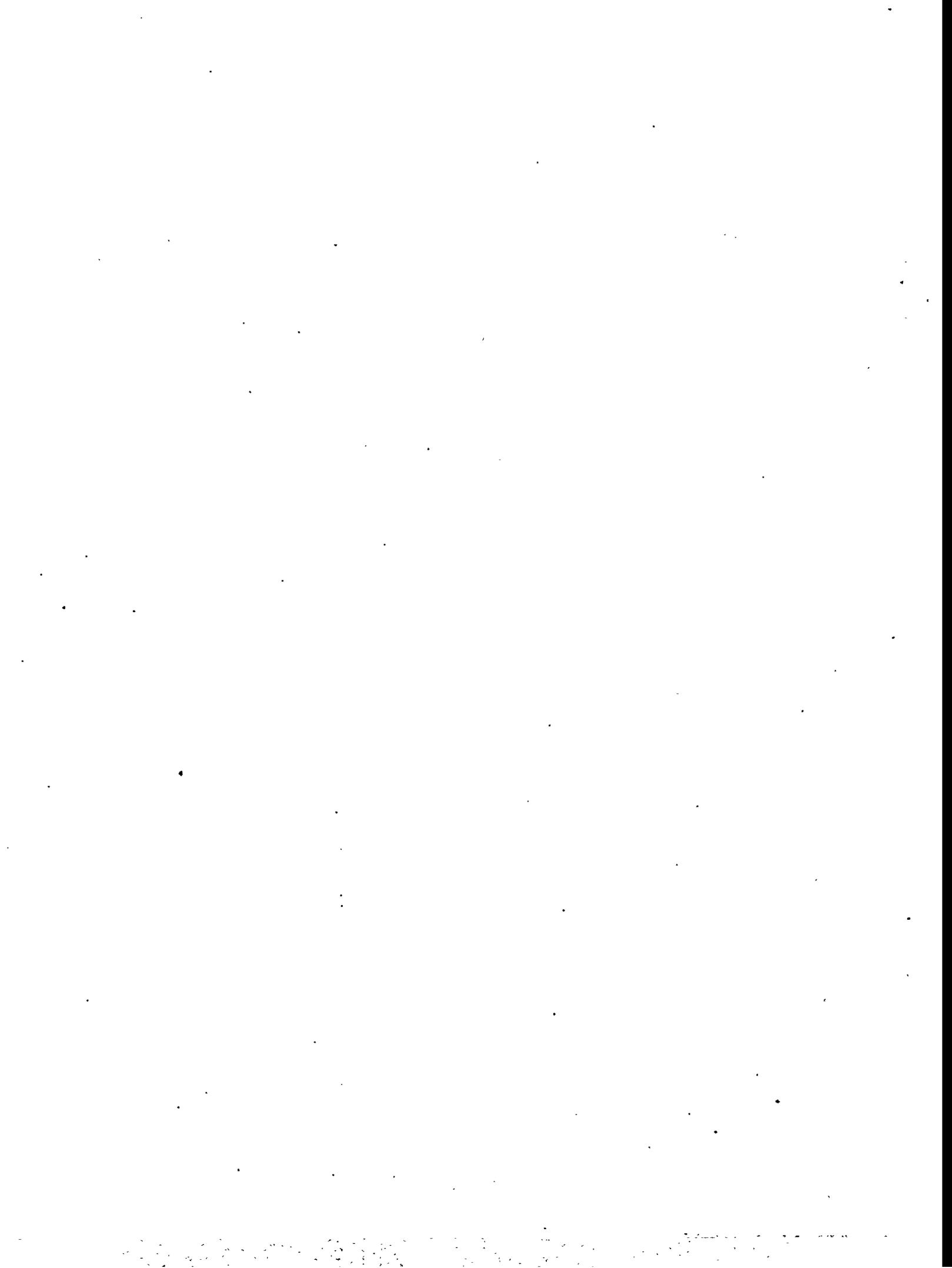
PREFACE

This report is one of a series of reports that document the mathematical models in the Multimedia Environmental Pollutant Assessment System (MEPAS). Developed by Pacific Northwest National Laboratory^(a) for the U.S. Department of Energy, MEPAS is an integrated impact assessment software implementation of physics-based fate and transport models in air, soil, and water media. Outputs are estimates of exposures and health risk assessments for radioactive and hazardous pollutants.

Each of the MEPAS formulation documents covers a major MEPAS component such as atmospheric, vadose zone, groundwater, surface water, overland, and exposure/health impact assessment. Other MEPAS documentation reports cover the sensitivity/uncertainty formulations and the database parameter constituent property estimation methods. The MEPAS atmospheric component is documented in this report.

MEPAS simulates the release of contaminants from a source, transport through the air, groundwater, surface water, or overland pathways, and transfer through food chains and exposure pathways to the exposed individual or population. For human health impacts, risks are computed for carcinogens and hazard quotients for noncarcinogens. MEPAS is implemented on a desktop computer with a user-friendly interface that allows the user to define the problem, input the required data, and execute the appropriate models for both deterministic and probabilistic analyses.

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SUMMARY

The Multimedia Environmental Pollutant Assessment System (MEPAS) is an integrated software implementation of physics-based fate and transport models for health and environmental risk assessments of both radioactive and hazardous pollutants. This atmospheric component report is one of a series of formulation reports that document the MEPAS mathematical models.

MEPAS is a "multimedia" model; pollutant transport is modeled within, through, and between multiple media (air, soil, groundwater, and surface water). The estimated concentrations in the various media are used to compute exposures and impacts to the environment, to maximum individuals, and to populations.

The MEPAS atmospheric component for the air media documented in this report includes models for emission from a source to the air, initial plume rise and dispersion, airborne pollutant transport and dispersion, and deposition to soils and crops. The material in this report is documentation for MEPAS Versions 3.0 and 3.1 and the MEPAS version used in the Remedial Action Assessment System (RAAS) Version 1.0.

The atmospheric component of MEPAS uses a series of climatological models for modeling the releases from point and area sources. In MEPAS, emission estimation models are provided as an alternative method for cases where the emission rates are unknown or cannot be back-calculated from environmental monitoring data. MEPAS has seven volatilization models for estimating gaseous vapor emissions from various types of sources and a particle suspension model for estimating soil-bound pollutant emissions. Plume rise models are included for stack releases. A sector-average Gaussian model using standard dispersion rates is used for the atmospheric transport. Both wet and dry deposition are computed. An important enhancement is that the wind speed, dispersion, and deposition models account for the influence of local surface roughness. This feature allows the model to account for local roughness influences along a wind trajectory ranging from smooth over-water to

rough forest cover. A complex-terrain nocturnal flow option allows for the near-source channeling of airborne releases.

The major products from these atmospheric component models include 1) contaminant emission rates, 2) regional patterns of long-term air concentrations and deposition rates normalized by emission rates, 3) near-release short-term acute air concentrations normalized by emission rates, 4) long-term deposition rates for selected types of surfaces, and 5) regional patterns of ambient pollutant concentrations. These output products from the atmospheric component are linked as input to other components as part of the integrated MEPAS exposure and impact evaluation software.

ACKNOWLEDGMENTS

The development of this multimedia contaminant environmental exposure and risk assessment methodology over the past decade required input from a wide spectrum of engineering and scientific technologies. The original MEPAS concept was developed by G. Whelan and B. L. Steelman. They were joined by K. A. Higley, D. L. Strenge, B. L. Hoopes, and the authors of this volume to form the initial MEPAS development team.

The development of the air component of MEPAS involved a number of staff. D. L. Strenge, and B.L. Hoopes helped in the initial design and integration with other components. C. D. Whiteman provided input on processes in complex terrain. S. Hwang, J. L. Stroh, and G. P. Streile provided inputs on volatilization models. C. J. Fosmire helped in the implementation of the formulations presented in this document.

We also wish to acknowledge L. J. Thibodeaux for his helpful suggestions and lecture notes relative to the modeling of volatilization from ponds.

We also acknowledge valuable inputs from the following review efforts: U. S. Department of Energy's (DOE) Environment Survey MEPAS External Peer Review Panel, U. S. Environmental Protection Agency's Review of Hazard Ranking Systems, Health and Welfare Canada's Review of Multimedia Models, Hanford Single Shell Tanks Review Panel conducted by the National Academy of Sciences, DOE's Environmental Restoration Priority System External Review Panel, the DOE Programmatic Environmental Impact Statement External Review Panel, and U. S. Department of Defense's Review of Risk Prioritization Methodologies conducted by the National Academy of Sciences.

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1.0 ATMOSPHERIC PATHWAY

Pacific Northwest National Laboratory (PNNL) prepared this report for the U.S. Department of Energy (DOE). This report describes the atmospheric pathway component of the Multimedia Environmental Pollutant Assessment System (MEPAS), including the purpose and use of the component's modules and formulations. This document replaces earlier MEPAS formulation documents (Whelan et al. 1987; Droppo et al. 1989). The atmospheric pathway component modules, formulations, and rationale are discussed in the following sections:

- emission characterization, including particle suspension and volatilization
- contaminant transport, dispersion, and deposition, including dispersion coefficients
- initial source dispersion, including point and area sources, wind conditions, radioactive decay, chemical reactions, wet and dry deposition, source mass budget, and plume rise
- air-as-source, short-distance, disperse-regional-release, and complex-terrain modules.

The atmospheric pathway component of MEPAS estimates the pollutant exposures from atmospheric emissions to a regional human population. Long-term, average contaminant levels are computed using standard computation techniques for locations defined in terms of a direction and distance from the site. Using these methods, estimates of contaminant levels for exposure assessment can be made for both population centers and less populated rural areas. Short-term normalized air concentrations are provided for evaluation of acute exposures at nearby locations.

1.1 LONG-TERM AVERAGE EXPOSURE

The long-term average exposure in the atmospheric pathway, based on a 70-year increment (i.e., approximately one human life span), represents the sum of exposures from individual atmospheric plumes. The travel time between

release and exposure for these individual plumes is typically expressed in hours and minutes. Therefore, relatively short-term processes need to be incorporated into the computation of long-term, average concentrations.

Modeling the long-term, average exposures to pollutants in the atmospheric pathway involves a weighted summation of exposures computed for a matrix of cases spanning ranges of ambient atmospheric conditions. The average conditions over the 70-year exposure period are represented by climatological data summaries (i.e., average frequency of occurrence of the various combinations of ambient atmospheric conditions) from a source such as the U.S. National Weather Service.

1.2 SHORT-TERM AVERAGE EXPOSURE

The short-term exposure to pollutants in the atmospheric pathway is based on maximum hourly concentrations. For a near-ground-level release, the 95% and 50% normalized air concentrations at 100 m from the release are provided. For all types of atmospheric releases, the maximum hourly normalized air concentration and its location are provided for each of the 16 direction sectors.

1.3 ATMOSPHERIC PROCESSES

The fate of a contaminant released to the atmosphere depends on a number of complex processes including release mechanisms and characteristics, dilution and transport, chemical reactions, washout by cloud droplets and precipitation, and deposition onto the underlying surface cover. The MEPAS atmospheric pathway model accounts for each of these processes in computing long-term exposures. A schematic diagram illustrating the atmospheric pathway is presented in Figure 1.1.

The atmospheric pathway for pollutants considers contaminant air concentrations and deposited surface concentrations. Air concentrations are needed for inhalation pathways. Surface concentrations resulting from dry and wet

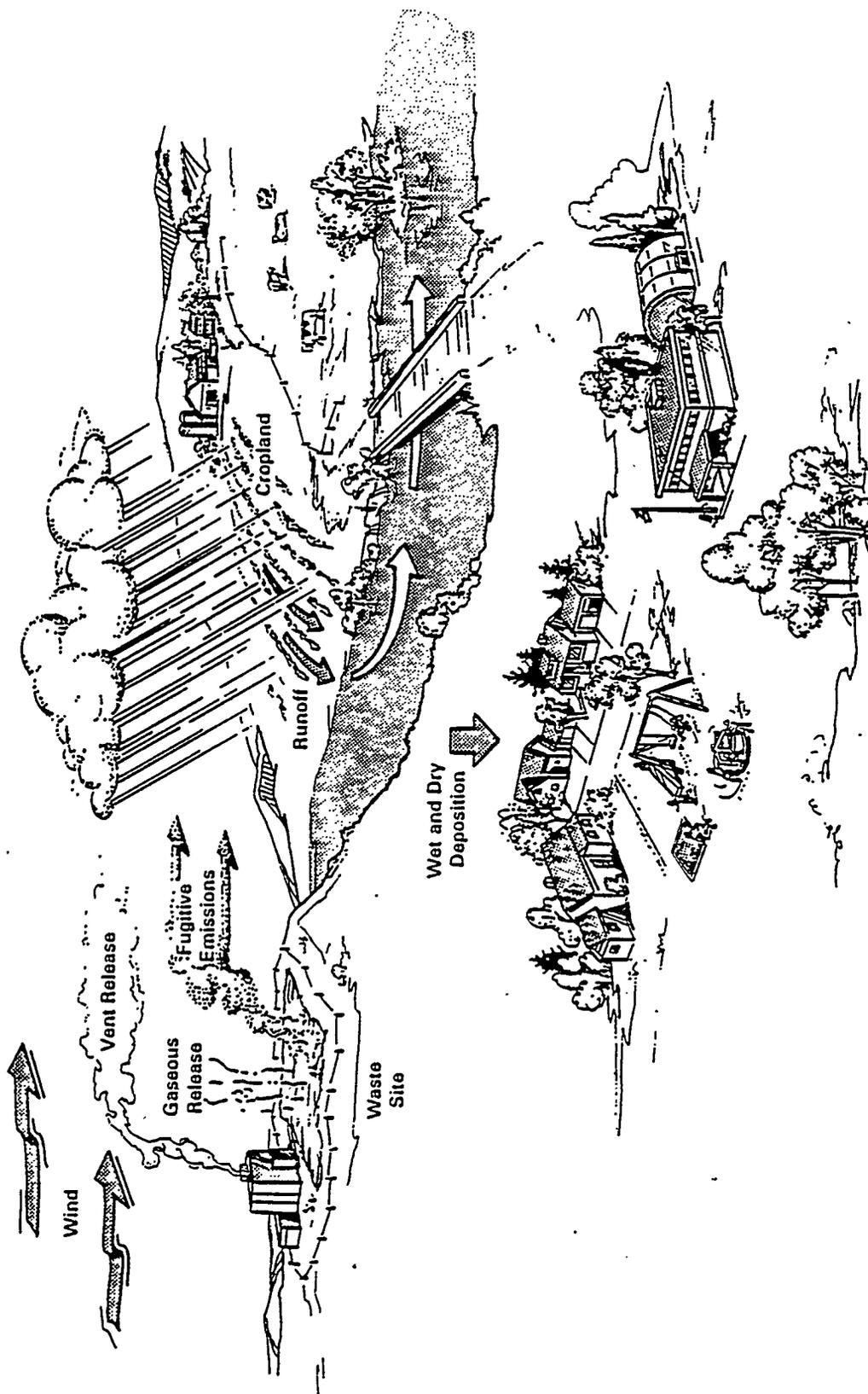


FIGURE 1.1. Schematic Diagram Illustrating the Atmospheric Environment

removal processes are needed for overland transport and for ingestion pathways for pollutants.

The atmospheric pathway has several sequential components: suspension/emission, atmospheric transport and dispersion, and wet and dry deposition. The relationship of these atmospheric components in the MEPAS model is shown in Figure 1.2. If using a MEPAS emission module, site-specific data are needed to estimate the gaseous and particulate release rates. An atmospheric transport and dispersion model is used to compute downwind air concentrations. As the plume travels away from a site, these airborne concentrations are reduced both by dispersion and deposition processes. Wet- and dry-deposition models are used to compute the total deposition to the surface. These atmospheric pathway components maximize the validity of comparisons of environmental trends between sites by being based on empirical relationships that incorporate site characteristics (i.e., location, surface cover, climatology).

The prediction of contaminant movement through the atmospheric pathway uses algorithms that address atmospheric suspension/emission of contaminants at a site and the subsequent transport, diffusion, and deposition of these airborne contaminants. Input to the model includes site-specific climatological information such as wind speed and direction, stability, and precipitation. Output from the model consists of average air and surface contaminant levels that are used in both the inhalation and ingestion components of the exposure assessment analysis. The computed surface contaminant levels also can be input to the overland transport components of MEPAS as a separate analysis run.

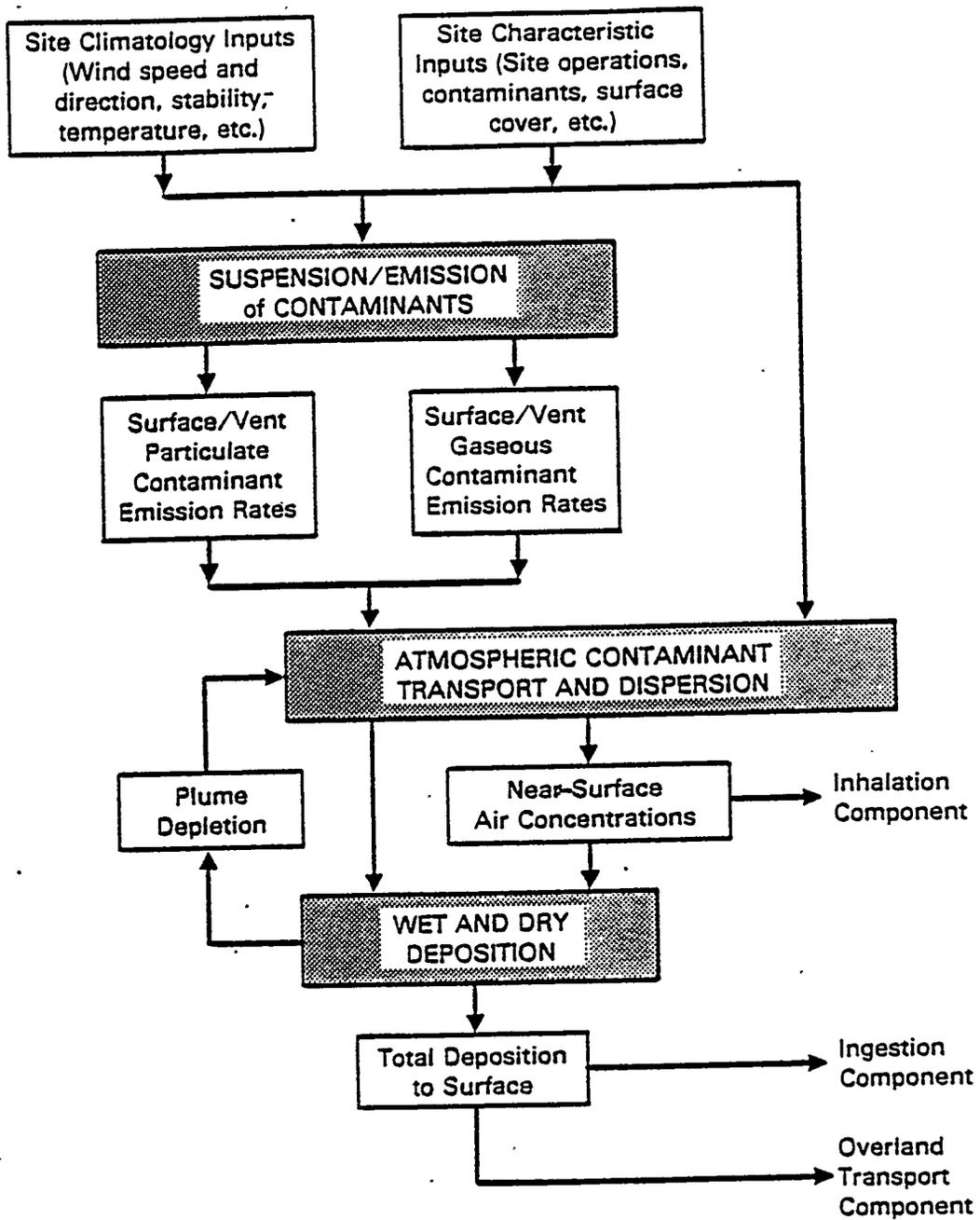
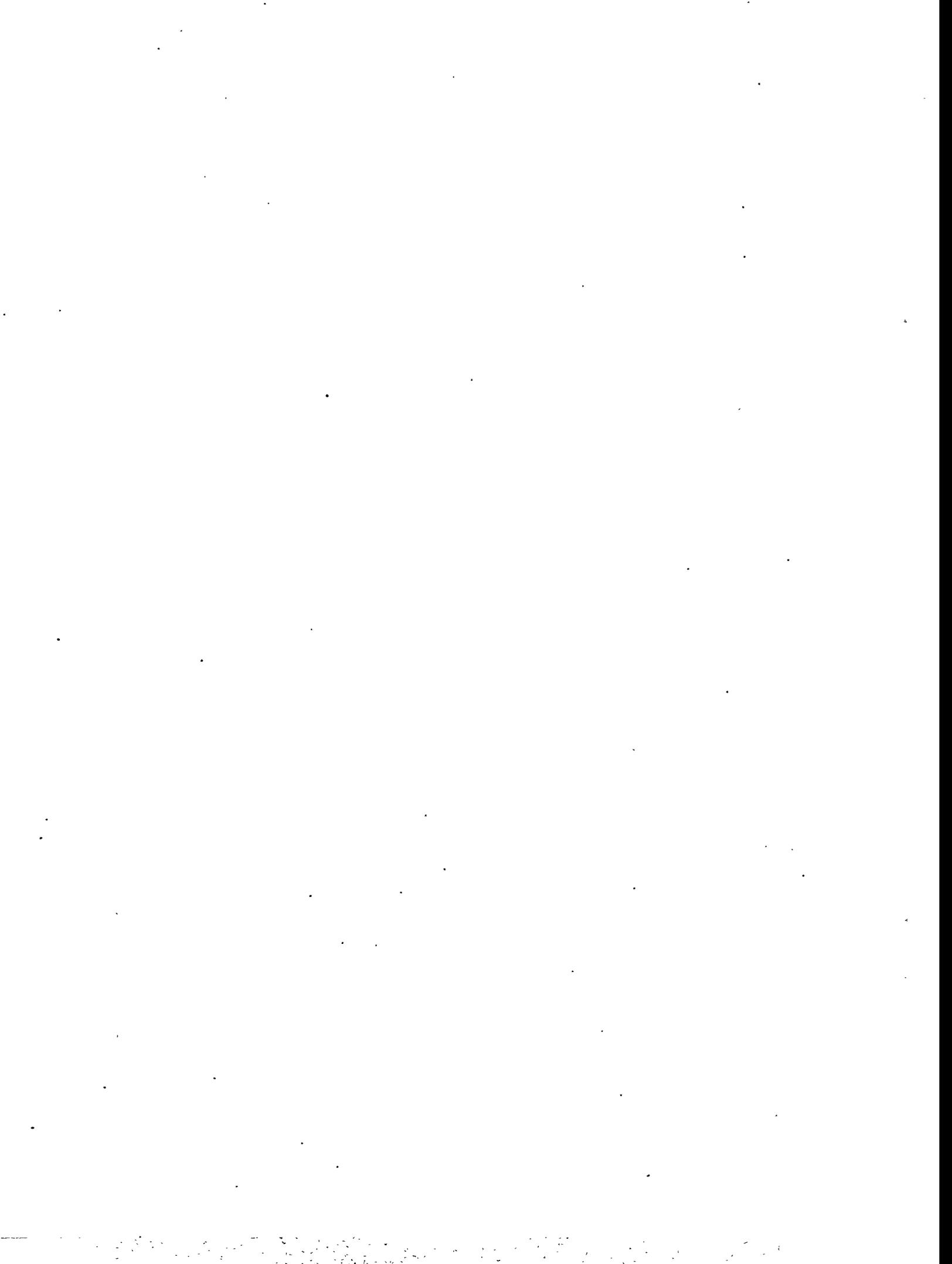


FIGURE 1.2. Atmospheric Pathway Computation Diagram



2.0 EMISSION CHARACTERIZATION

Atmospheric releases of pollutants may occur by a number of mechanisms such as volatilization, suspension, leakage, and direct emission. These releases may be characterized as being from either area sources (e.g., surface contamination, landfills, lagoons) or point sources (e.g., stacks, vents).

The emission formulations in this document refer to MEPAS Version 3.1 which limits the total emissions to the air based on a contaminant mass budget for the air emissions. This report does not specifically address the MEPAS multimedia source term component.^(a)

The MEPAS atmospheric component supports several methods for defining atmospheric release rates:

- For both point sources and area sources the investigator may input the release rate of contaminants.
- For area sources, the investigator may input site characteristics and have MEPAS compute the pollutant release rates associated with the suspension of particulates and emission of gases (volatilization).
- For both point and area sources, the investigator may use long-term environmental monitoring data to back-calculate an apparent pollutant release rate.

The release of contaminants into the atmosphere is often a function of local conditions. Important factors can be temperature, moisture, wind speed, surface characteristics (e.g., crust formation, roughness, vegetation cover), the physical state and chemical form of the contaminant (e.g., gas or particulate, reactive or nonreactive), and location of the contaminant (i.e., on the surface, buried under a soil layer, in a tank). The formulations for com-

(a) The multimedia source term component is being developed at the time of preparation of this report. This new component combines source computations of emissions to water, soil, and air to compute an integrated time-dependent mass budget. A separate document will be issued with the multimedia source term component formulations.

puting pollutant release rates from site characteristics are described in this chapter.

2.1 SUSPENSION OF SURFACE PARTICLES

Particulate fugitive releases of contaminants are defined as emissions resulting from suspension of exposed surface contamination by wind or mechanical processes to the air. If a site has exposed surfaces with contamination, the potential suspension of the contaminants depends on factors such as the physical and chemical surface characteristics, surface contamination, ambient wind speed, turbulence, and local mechanical activity on the surface.

A surface cover with contaminants may be the result of either waste storage (e.g., mill tailings) or contamination by the operation of a facility. The latter contamination may occur on natural surfaces (e.g., soil) or artificial surfaces (e.g., concrete pads, roadways). The potential for suspension of contaminants varies greatly because of the wide variety of surface types and activities expected on the surfaces.

The suspension of particles from the surface may occur as the result of wind action (Bagnold 1941; Sehmel and Lloyd 1976) or other physical action on the surface (Sehmel 1976). Atmospheric turbulence plays a role in determining the extent to which the air movement over the surface can suspend surface particles. Local mechanical activity on the surface, such as animal grazing, vehicular traffic, walking, and earth moving can greatly increase the fugitive particulate release rates compared to an undisturbed surface.

The suspension of respirable particles (particles with diameters less than 10 μm) from contaminated areas at DOE sites is calculated using empirical relationships based on studies of wind erosion and surface disruption. The MEPAS outputs for suspension from contaminated surface areas are expressed in

terms of an airborne soil concentration normalized to a unit surface contamination. These soil concentration arrays are converted to arrays of contaminant concentrations using the fraction of surface contamination in the suspended soil.

Computing the suspension of contaminants from a surface into the atmosphere requires both contaminant and site data. These data are used to define which formulations, if any, apply to the site. If a computation is appropriate, these data are used to compute the suspension rates.

The MEPAS methodology for computing suspension rates is an adaptation of the methodology proposed by Cowherd et al. (1985) for rapid computation of potential long-term impacts from spills of hazardous materials. This methodology which includes formulations for contaminant suspension by winds, vehicular traffic, and other physical disturbances of the surface, is similar to, but not identical to, the U.S. Environmental Protection Agency's (EPA) AP-42 revision of the Cowherd et al. (1985) model for industrial wind erosion (EPA 1988a, 1995).

2.2 WIND EROSION AND MECHANICAL SUSPENSION

Cowherd et al. (1985) define the steps for determining potential respirable particulate emission from wind erosion. The soil particle size distribution, apparent roughness of the site, vegetation cover, presence of a crust on the soil, and presence of nonerodible elements (e.g., large stones) are used to define the potential for suspension. Depending on the results of their procedure, the site is characterized as having 1) unlimited erosion potential, 2) limited erosion potential, or 3) no erosion potential.

The methodology uses different formulations for the two cases with wind erosion potential. Cowherd et al. (1985) suggest that if the site is completely covered with vegetation or if there is a thick crust (or a wet, saturated soil) and if no mechanical disturbances occur at the site, it can be assumed that no contaminants are suspended. However, for certain contami-

nants, even very small suspension rates from well-stabilized surfaces may be significant. These wind erosion formulations give results comparable to using resuspension factors over a range of surfaces from bare, unstabilized surfaces to well-stabilized surfaces (Whelan et al. 1989).

The potential for wind erosion is quantified in terms of a threshold friction velocity. The greater the value of the threshold friction velocity for a site, the lower the potential for particle suspension. The threshold friction velocity for the contaminated area is determined by knowing the mode of the aggregate particulate size distribution (which is derived from the soil composition) and using a formula derived from the graphical relationship given by Gillette et al. (1980):

$$u_c^* = \frac{N \exp[0.4118428 \ln (X) + 0.04167173]}{100} \quad (1)$$

- where u_c^* = threshold friction velocity (m/s)
 X = aggregate size distribution (mm)
 N = nonerodible elements correction factor (dimensionless).

The aggregate size distribution is estimated using $X = (0.0106)(\text{Percent Sand}) + 0.05$. From the viewpoint of increasing the potential for suspension, this relationship provides relatively realistic estimates for soils with greater than 75% sand content. For other soils, the relationship provides relatively conservative estimates that are more typical of disturbed soils than undisturbed soils.

The correction factor in Equation 1 allows for the effects of any non-erodible elements in the contaminated area. This correction factor for the fraction of surface coverage is estimated on graphical results given by Cowherd et al. (1985), derived from wind tunnel studies by Marshall (1971). As the silhouette area of nonerodible elements increases, so does the threshold friction velocity. If the threshold friction velocity is less than 0.75 m/s, the area has unlimited erosion potential; otherwise, the area has

only limited erosion potential. In MEPAS, the emission rate for a surface is computed as the sum of the unlimited and limited erosion emissions. The emission rate terms were not summed in the original methodology described by Cowherd et al. (1985).

Once the threshold friction velocity has been determined, the critical wind speed at a given height above the surface can be determined using the equation

$$u' = \frac{1}{r} u_c^* \ln(z/z_0) \quad (2)$$

where u' = critical wind speed at 7-m height (m/s)

r = von Karman constant (0.4; dimensionless)

z = reference height above the surface (7 m)

z_0 = surface roughness length (m).^(a)

The critical wind speed is one of the parameters used below to define the erosion potential. The value of z recommended by Cowherd et al. (1985) is 7 m. The surface roughness length of the site, z_0 , is related to the size and spacing of the roughness elements in the area. Figure 2.1 illustrates z_0 for various surfaces (Cowherd and Guenther 1976).

For estimating particulate emissions from a contaminated area having limited wind-erosion potential, the following equation is used to predict potential emissions:

(a) Units for the surface roughness length are listed as meters (m) for consistency in Equation 1; the common units for this variable are centimeters (cm) as presented in Figure 2.1.

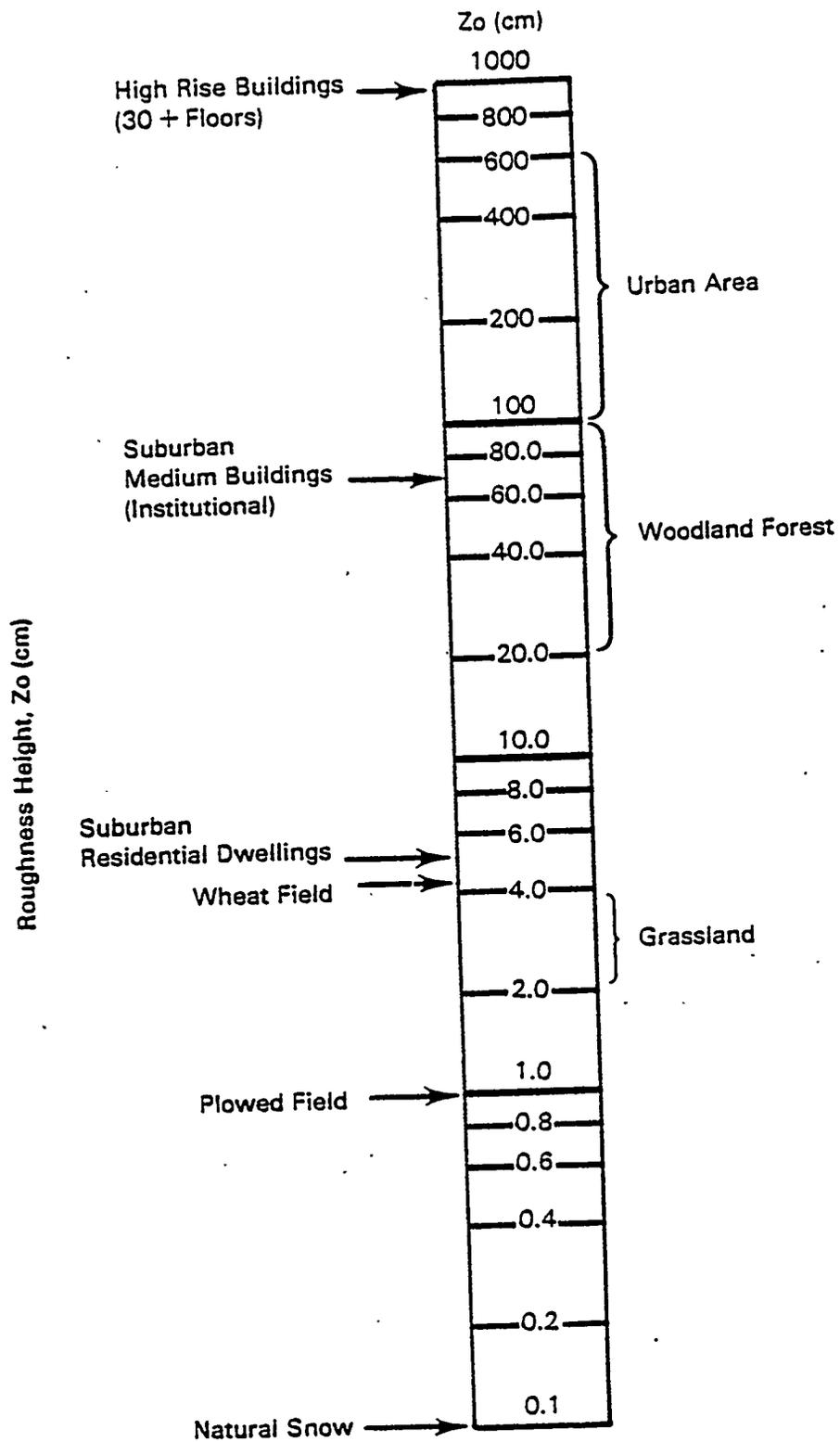


FIGURE 2.1. Roughness Lengths for Various Surfaces (Cowherd et al. 1985)

$$E_{10} = 8.3 \times 10^{-4} \left[\frac{f p(u) (1 - v)}{\left(\frac{PE}{50}\right)^2} \right] \quad (3)$$

where E_{10} = annual average emission rate per unit surface area ($\text{g}/\text{m}^2/\text{hr}$)

f = frequency of mechanical disturbances (number/months)

u = observed maximum wind speed for periods between disturbances corrected to a reference height of 7 m (m/s)

$p(u)$ = erosion potential (g/m^2)

v = vegetation coverage on surface (fraction)

PE = Thornthwaite's Precipitation-Evaporation (PE) Index (dimensionless).

The frequency of disturbances per month, f , is defined as the number of actions that could expose fresh surface material. If the entire area is not disturbed, this frequency should be weighted to reflect the actual area exposed. A disturbance could be vehicular traffic, plowing or turning of the soil, mining, or construction. The erosion potential, $p(u)$, depends on the maximum wind speed, u , so that

$$\begin{aligned} p(u) &= 6.7 (u - u') & \text{if } u \geq u' \\ p(u) &= 0.0 & \text{if } u < u' \end{aligned} \quad (4)$$

The vegetation fraction varies from 0 for bare ground to 1 for total coverage. The Thornthwaite's PE Index is used as a moisture-correction parameter for wind-generated emissions. Cowherd et al. (1985) provide a map with values of PE for all regions in the contiguous United States (Figure 2.2).

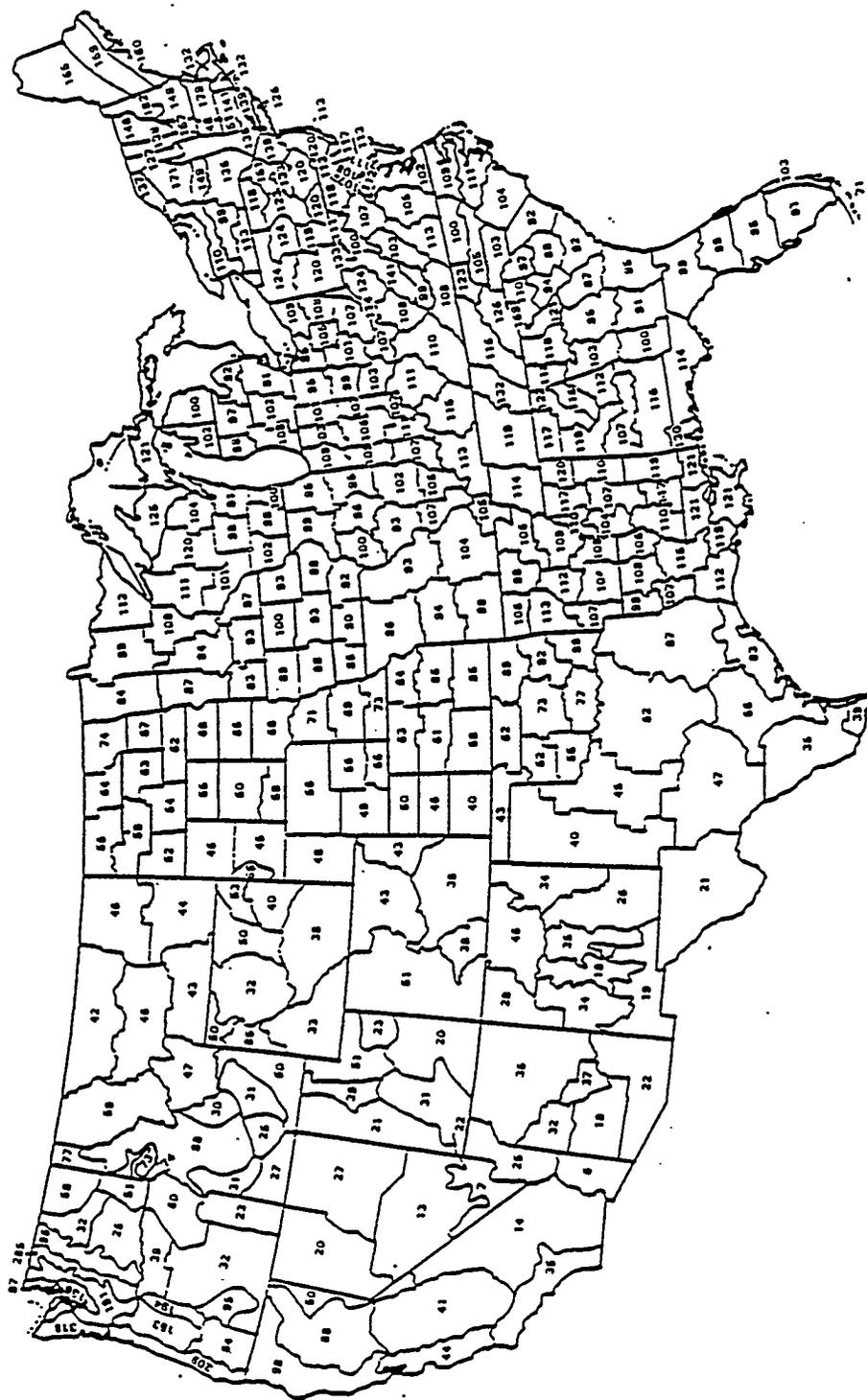


FIGURE 2.2. Map of Precipitation-Evaporation Index for State Climatic Divisions (Cowherd et al. 1985)

For unlimited erosion potential, the relationship for the surface emission rate is

$$E10_u = 0.036(1 - v) \left[\frac{\bar{u}}{u'} \right]^3 F(x) \quad (5)$$

where \bar{u} = mean annual wind speed (m/s)

$F(x)$ = integration function

$E10^u$ = annual average emission rate per unit surface area (g/m^2).

The vertical flux of particles smaller than 10 μm in diameter is assumed to be proportional to the cube of the horizontal wind speed. This relationship was originally developed from measurements made by O'Brien and Rindlaub (1936) in studies at the mouth of the Columbia River and later measurements made by Bagnold (1941) in the Egyptian desert. Chepil (1951) found this same relationship using results from wind-tunnel experiments.

The integration function, $F(x)$, comes from the cubic relationship of the vertical transport of particles and the wind speed. It is defined in graphical format by Cowherd et al. (1985). This relationship can be broken into the following discrete parts:

$$\begin{array}{ll} F(x) = 0.0 & \text{if } x < 0.0 \\ F(x) = 1.91 & \text{if } 0.0 \leq x < 0.5 \\ F(x) = 1.9 - (x - 0.5) 0.6 & \text{if } 0.5 \leq x < 1.0 \\ F(x) = 1.6 - (x - 1.0) 1.3 & \text{if } 1.0 \leq x < 2.0 \\ F(x) = 0.18x(8x^2 + 12)e^{-x^2} & \text{if } 2.0 \leq x \end{array} \quad (6)$$

where $x = 0.886 u' / \bar{u}$.

2.3 VEHICULAR SUSPENSION OF PARTICLES

Formulations used to compute pollutant emissions per unit area resulting from the mechanical disturbances by vehicle traffic are also based on Cowherd et al. (1985). The pollutant emission caused by traffic moving over unpaved surfaces is computed using

$$E10 = (0.85) \left[\frac{s}{10} \right] \left[\frac{S}{24} \right]^{0.8} \left[\frac{W}{7} \right]^{0.3} \left[\frac{w}{6} \right]^{1.2} \left[\frac{365 - p}{365} \right] \quad (7)$$

where E10 = emission factor for an unpaved surface expressed as mass suspended per vehicle-kilometer of travel [g/(vehicle-km)]

s = silt content of road surface material (%)

S = mean vehicle speed (km/hr)

W = mean vehicle weight (Mg)

w = mean number of wheels

p = number of days with at least 0.254 mm (0.01 in.) of precipitation per year.

Site-specific information from local sources is normally obtained for each of the parameters. When site-specific data are not available, the default values given by Cowherd et al. (1985), which are listed in Table 2.1, may be used.

Values for p are obtained from a local source of meteorological data.

TABLE 2.1. Default Values for Independent Variables of Equation 7^(a,b)

Site	s(%)	S(km/hr)	W(Mg)	w
Rural/Residential	15 (5-68)	48 (40-64)	2	4
Industrial	8 (2-29)	24 (8-32)	3	4
			15	6
			26	10

(a) Based on Cowherd et al. (1985).

(b) Numbers in parentheses are ranges of measured values.

2.4 EMISSION RATE COMPUTATION

Once the various emission factors for particle suspension have been determined, the emission rates for respirable particles can be calculated. For wind erosion and mechanical suspension, the emission rate is calculated from the relationship

$$R_{10} = E_{10} \text{ area} \quad (8)$$

where R_{10} = emission rate for wind erosion (g/s)

area = area of source contamination (m^2).

A climatological suspension factor, used in Cowherd et al.'s (1985) original formulation, corrected the dispersion values in their workbook for the fraction of suspension time. That factor is not needed in the MEPAS implementation that computes site-specific dispersion values.

For mechanical suspension of particles from vehicle traffic on an unpaved contaminated surfaces, the emission rate is computed from

$$R_{10} = (1.157 \times 10^{-5}) E_{10} L T \quad (9)$$

where R_{10} = emission rate caused by traffic (g/s)

L = distance of travel over contaminated surface (km)

T = average number of vehicles traveling over the contaminated surface per day (number/day).

For a paved road, the assumption is made that 1% of the road is covered with respirable material.

The total emission rate is the sum of the wind-erosion and mechanical-disturbance emission rates. The total emission rate is used as input to the atmospheric dispersion, transport, and deposition model.

Subsequently, the airborne and surface pollutant concentrations resulting from the suspension of a specific surface contaminant, θ , are computed using the following equations:

$$C_{\theta} = \alpha C_s \quad (10)$$

and

$$S_{\theta} = \alpha S_s \quad (11)$$

where C_{θ} = airborne contaminant concentration (g/m^3)

C_s = airborne soil concentration (g/m^3)

α = mass fraction of contaminant in the suspended surface soil (g/g)

S_{θ} = surface concentration of deposited contaminant (g/m^2)

S_s = surface concentration of deposited soil material (g/m^2).

2.5 VOLATILIZATION

When hazardous materials are in accident, disposal, or storage areas such as landfills, spill sites, contaminated soil, and ponds, the volatile

constituents may be emitted directly to the air in a gaseous form. The processes by which this exchange of gaseous materials to the air occurs is called volatilization.

The volatilization pathway can dominate the potential human health impacts of an environmental problem. A typical example of this kind of problem is a landfill with volatile organic compounds that result in significant exposures from inhaling these vapors. In addition, semivolatile emissions of materials, such as PCBs, can be important sources of pollutant exposure via the volatilization pathway (EPA 1988b).

MEPAS provides three methods to address volatilization. The gaseous release rates may be

- input by the investigator
- computed by the model
- back-calculated from air concentration monitoring data.

For the input method, emission rates are obtained from sources such as flux measurements at the contaminant source, or computation with an alternative volatilization model. The computation method requires input of site-specific information on the constituent and site characteristics. The back-calculation method using monitoring data requires information on the size of the contaminated area and ambient concentrations.

The mathematical formulations for estimating atmospheric volatilization rates are described in the following sections. Gaseous emissions of constituents from landfills, spills, and ponds are computed using physical characteristics of the contaminant source and chemical properties of the contaminants.

A number of models have been proposed and summarized for computing volatilization rates from soils and ponds with liquid mixtures of waste (see EPA 1980; Farino et al. 1983; Thibodeaux 1981; Shen 1981; Thibodeaux and Hwang 1982; Mackay and Leinoen 1975; Lyman et al. 1982; and Hwang and Falco 1986 as

cited in EPA 1990). Different models have been developed to estimate emission rates from different types of treatment and disposal activities. The MEPAS volatilization mathematical formulations include models published in the literature for estimating emission rates of volatile compounds from soils, various treatment and disposal facilities, and spill sites. Knowledge of the derivation of a model is important in selecting an appropriate model to best represent the condition of the contaminants, the media from which emissions occur, and their interactions at a specific site. Because of many similarities among these models, it is important to understand the assumptions made by the authors in deriving these models.

MEPAS includes mathematical formulations for computing volatilization rates from several different types of contaminant sources based on the U.S. Environmental Protection Agency's (EPA's) recommendations in the Superfund Exposure Assessment Manual (EPA 1988b) and a guidance document (EPA 1990). The MEPAS volatilization source models are for contamination in soil and liquids:

- contaminated soil gradient model (soil)
- land treatment facilities (soil)
- landfills without internal gas generation (soil)
- landfills with internal gas generation (soil)
- spill sites (pooled liquid)
- surface impoundments (liquid storage).

Note that the first three models are all applicable to soil contamination. The formulations given below should be used to help determine which source model applies best to a particular soil contamination situation.

2.6 CONTAMINATED SOIL MODELS

Contaminated soil can be caused by leaks or spills of hazardous liquid or solid materials, or improper treatment, storage, or disposal of the such

materials. Volatile components contained in the soil medium can be a major source of pollutant air emissions. The degree of volatile emissions from soil will depend upon the type of the contaminant, the chemical and physical properties of the contaminant, and the physical characteristics of the medium and the site.

The rate of volatile emission from contaminated soil may be increased by remediation activities. Old hazardous waste sites containing volatile constituents may not emit vapors in significant amounts, but disturbing the soil in the process of remediation can redistribute the concentration profile across the soil depth, and can increase emission rates from the soil significantly.

2.6.1 Contaminated Soil Gradient Model

Hwang and Falco (1986) developed a model for estimating emission rates of volatile and semivolatile components in soil by solving a partial differential equation describing the process of diffusion and partitioning occurring within the soil. The solutions are presented for two cases: one case for predicting the emission rate from soil when there is no clean cover on top of soil and another case for predicting the emission rate when a clean soil cover is applied on top of soil immediately after remediation.

2.6.2 Contaminated Soil Gradient Model Without A Clean Soil Cover

This model based on Hwang and Falco (1986) is implemented as a volatilization source model referred to as "Contaminated Soil" (AG-VCASE = 5) in the user-interface of MEPAS 3.n versions. The "Contaminated Soil" model is one of the models recommended by the EPA (1990) for estimating emission rates from contaminated soil as part of the Superfund exposure and risk assessment process.

The physical basis of the model is as follows. The contaminant in the soil is assumed to be initially distributed uniformly across the soil depth and across the depth up to the surface (e.g., without a clean soil cover on the surface). As emissions occur from the soil surface, the concentration gradient across the depth in the vertical direction is established. This

concentration gradient limits the emission rate as time elapses. Under these conditions, Hwang and Falco (1986) present the following model for estimating the transient volatilization rate at some time, t:

$$N_i = \frac{\epsilon D_{ei}}{\sqrt{\pi \alpha t}} \frac{H_c}{K_d} C_{so} \quad (12)$$

where N_i = emission rate of contaminant i per unit surface area (g/cm²/s)

ϵ = air-filled porosity of soil (dimensionless)

D_{ei} = effective diffusivity defined as $D_i \epsilon^{1/3}$ (cm²/s)

D_i = molecular diffusivity of contaminant in soil air pore (cm²/s)

H_c = concentration-based Henry's Law constant, or concentration in air/phase/concentration in water phase (dimensionless), which is computed as $H / R T$

H = Henry's Law constant (atm m³/mole)

R = gas constant (8.2 x 10⁻⁵ atm m³/°K-mole)

T = temperature (°K)

K_d = soil-water partition coefficient (cm³/g)

t = time (s)

C_{so} = initial (t=0) contaminant concentration in soil (g/g)

α = a term defined as $(D_{ei} \epsilon / [\epsilon + P_s (1-\epsilon) K_d / H_c])$ (cm²/s)

P_s = true density of soil, g/cm³.

The emission rate estimated by Equation 12 represents an instantaneous emission rate at any time t. The emission rate shown by this equation decreases as a function of time. The emission rate averaged over a long-term period can be obtained mathematically by integrating the instantaneous emission rate over the exposure period and dividing it by the exposure period.

The result is

$$\bar{N}_i = 2 N_i \quad (13)$$

The total average emission is obtained by multiplying the emission rate in Equation 13 by the emission area,

$$E_i = 2 N_i A \quad (14)$$

where E_i = emission rate of constituent i (g/s)

A = emission area (cm^2).

The emission rate from soil contaminated by organic compounds can be estimated from Equation 12 where the soil-air partition coefficient is defined by H_c/K_d and the value for K_d is related to the value of the octonal-water partition coefficient, K_{oc} . In some special cases where the K_{oc} values are not known and the compounds exert vapor pressures, Equation 12 can be modified to estimate the emissions. Examples of these special cases include soil contaminated with mercury or tritiated water in a mixture with water. Vapor pressures of the compounds in the soil pores provide a driving-force for air emissions and the driving-force term, $(H_c/K_d) C_{so}$, requires modification to estimate the transient emission rate. The term, $(H_c/K_d) C_{so}$, represents the concentration of a contaminant in the air space of soil pore at the beginning of contamination, and hence can be replaced by

$$\left[\left[\frac{H_c}{K_d} \right] C_{so} \right] = \left[\frac{VP_i MW_i}{R T} \right] X_i \quad (15)$$

where VP_i = vapor pressure of constituent i (mmHg)

MW_i = molecular weight of constituent i (g/g-mole)

X_i = weight fraction of constituent i in soil (g/g).

2.6.3 Contaminated Soil Gradient Model With A Clean Soil Cover

Covering a contaminated soil site with a layer of clean soil may decrease the rate of volatile emissions. The extent to which the emission rate decreases depends upon several factors including the partitioning behavior of the contaminant between the soil and soil pore, volatility of the contaminant, the cover thickness, and contaminant diffusivity through the soil pores. For the case of having a clean soil cover, the partial differential equation describing the physical phenomena of the volatilization process could not be solved analytically at the appropriate boundary and initial conditions. Hwang and Falco (1986) presented the solution in form of a converging series using the techniques of the Fourier series.

$$\bar{N}_i = \frac{2(Hc/Kd) C_{so} \epsilon D_{ei}}{L T} \sum_{n=0}^{\infty} \left[\int_{t_1}^{t_2} \exp\left[-\frac{\alpha (2n+1)^2 \pi^2 t}{4 L^2}\right] dt \cos\left[\frac{(2n+1) \pi k}{2 L}\right] \right] \quad (16)$$

where L = depth to the bottom of contamination from the soil surface (cm), including the depth of clean soil placed on top of contaminated layer

T = period over which emission rates are averaged (s)

k = depth of clean soil cover (cm)

\bar{N}_i = average emission rate of contaminant i over the exposure period T which is equal to $t_2 - t_1$, $g/cm^2 \cdot s$; when the initial exposure occurs at $t_1 = 0$; the exposure period T is equal to t_2 in Equation 15, and the integration starts from 0 to t_2 .

Other terms in Equation 16 are as defined in Equation 12. The summation in Equation 16 can be estimated with a computer. At the date of publication of this report, the above model for contaminated soil with a layer of clean soil is not implemented in MEPAS.

2.7 LANDFILLS WITHOUT INTERNAL GAS GENERATION

Landfills are differentiated from contaminated soil; volatile or semivolatile organics tend to occur in concentrated form within the landfill. A good example would be a landfill with volumes of leaking drums containing volatile organics covered with a layer of soil. The "Landfill" model presented below is also different than the "Contaminated Soil" model described above in that the emission rate is assumed to have reached a steady-state condition and thus is not changing with time.

EPA's (1988, 1990) model for computing volatilization rates from "landfills without internal gas generation" is implemented in the user-interface (AG-VCASE = 1) of MEPAS 3.n versions. The model is based on Fick's first law of steady-state diffusion as developed by Farmer et al. (1978). Diffusion from the landfill to the atmosphere is assumed to occur from the reservoir of organic contaminants in the landfill through the landfill cover. The subsurface soil concentrations are assumed to be uniform. Processes such as biodegradation, transport in water, adsorption, and landfill gas production are not included in the model development; the diffusion of the constituents in the soil is assumed to be the controlling mechanism for vapor transport.

Farmer's original model was modified and simplified by EPA (1980), Farino et al. (1983), and Shen (1981). The simplification included the assumption that the soil was completely dry to provide maximum volatilization rates based on the fact that diffusion in the pores in air is greater than diffusion in the pores in water. The MEPAS implementation of this model uses an expression that allows for soil moisture and comparison of results based on factors such as climatological differences. This expression can be simplified to a dry soil condition if the situation warrants. The resultant equation for the steady-state volatilization rate is

$$E_i = D_i C_s i A P_s M_i / d_{sc} \quad (17)$$

where E_i = emission rate of constituent i (g/s)

D_i = diffusion coefficient of constituent i in air (cm^2/s)

C_{si} = saturated vapor concentration of constituent i (g/cm^3)

A = exposed area where emissions occur (cm^2)

P_s = the ratio of air-filled soil porosity to total soil porosity (dimensionless)

M_i = weight fraction of constituent i in the waste (g/g)

d_{sc} = effective depth of soil cover (cm).

Equation 17 assumes that there is a soil cover above waste through which diffusion progresses. When no cover is assumed, Equation 17 is inappropriate ($d_{sc} = 0$ implies an infinite emission rate). The soil moisture is accounted for by replacing the total soil porosity with a porosity ratio term. This replacement was originally suggested by Millington and Quirk (1961) and was summarized by Hwang (1982) for application to toxic air emissions. This ratio was defined as

$$P_s = \frac{(P_a)^{10/3}}{P_t^2} \quad (18)$$

where P_t is the total soil porosity (dimensionless) and P_a is the air-filled soil porosity (dimensionless). When it can be assumed that the soil is dry, then Equation 18 simplifies to

$$P_s = P_t^{4/3} \quad (19)$$

The total soil porosity and the air-filled porosity may be based on the soil types. The percentage sand, silt, and clay may be obtained from U.S. Soil Conservation Service reports. In the rare case where the soil is completely dry, the air-filled porosity becomes the total soil porosity, and P_s

given by Equation 18 applies as occurs in the original formulation of Equation 17. The total porosity for a dry soil is calculated as

$$P_t = 1.0 - \left[\frac{\beta}{P_s} \right] \quad (20)$$

where β is the bulk density of the soil (g/cm^3), and P_s is the particle density (g/cm^3), usually 2.65 for mineral material.

The air-filled porosity, P_a , can be calculated using the total soil porosity minus the soil's field capacity for water as noted in EPA (1988), Fenn et al. (1975), Lynsley et al. (1975), Eagleson (1970), Hanks and Ashcroft (1980), and Israelsen and Hansen (1962). The equation for computing air-filled porosity is

$$P_a = P_t - \theta \quad (21)$$

where θ is the soil's percent field capacity for water (dimensionless).

If the diffusion coefficient for the constituent is unknown, it can be calculated using the following empirical relationship (O'Connor and Muller 1980):

$$D_i = 1.9(MW_i)^{-0.6667} \quad (22)$$

where MW_i = molecular weight of constituent i (g/mole).

When the landfilled waste constitutes a pure material, the molecular weight, air temperature, and vapor pressure of a constituent are needed to compute the vapor-phase concentration, C_{si} , using an equation from EPA (1980):

$$C_{si} = \frac{VP_i MW_i}{RT} \quad (23)$$

where C_{si} = saturated vapor concentration of constituent i (g/cm^3)

VP_i = saturated vapor pressure of constituent i (mm Hg)

MW_i = molecular weight of constituent i (g/mole)

R = molar gas constant ($6.23 \times 10^4 \text{ cm}^3 \text{ mm Hg/}^\circ\text{K-mole}$)

T = annual average air temperature ($^\circ\text{K}$).

Equation 16 was originally presented by Farmer et al. (1978) based on an experiment conducted for diffusion of a pure compound through soil. Hexachlorobenzene was the material held on a reservoir for diffusion experiments.

2.8 LANDFILLS WITH INTERNAL GAS GENERATION

EPA's (1988, 1990) model for computing volatilization rates from "landfills with internal gas generation" is implemented in the user-interface (AG-VCASE = 2) of MEPAS 3.n versions. Landfills with biodegradable organic waste material content can generate internal gas which can greatly enhance the emission rates of all gases. A landfill with a combination of municipal and industrial waste disposed of in trenches, for example, can generate volatile gases that sweep out organic vapors when it emerges from the codisposed waste materials. Thibodeaux (1981) developed the following equations for estimating enhanced gaseous emission rates from gas-generating landfills; Hwang (1982) presented a procedure for estimating emission rates using these equations:

$$\frac{E_i}{A} = V_y \frac{C_i^* - C_{i0}}{\exp\left[\frac{d_{sc} V_y \tau}{D_i \epsilon}\right] - 1} + V_y C_i^* \quad (24)$$

where E_i = emission rate of constituent i (g/s)

- C_i^* = concentration of constituent i in the soil pore spaces (g/cm³)
 C_{i0} = concentration of constituent i at the soil-air interface (g/cm³)
 V_y = mean landfill gas velocity (cm/s)
 A = area of landfill (cm²)
 d_{sc} = depth of the cover material (cm)
 τ = tortuosity (square root of 3 [= 1.73] for spherical particles)
 ϵ = porosity of the cover material to be determined by $\epsilon = 1.73 \frac{p_a^{10/3}}{p_t^2}$.

Because the value for C_{i0} is not known, Hwang (1982) indicated that Equation 24 should be solved simultaneously with

$$\frac{E_i}{A} = (2.44 \times 10^4) k_{g,i} (C_{i\infty} - C_{i0}) \quad (25)$$

where $k_{g,i}$ = gas-phase mass-transfer coefficient of component i (cm/s)

$C_{i\infty}$ = concentration of component i in the air far away from the soil-air interface (g/cm³); normally equal to zero.

Equations 24 and 25 can be solved simultaneously to get an expression for C_{i0} that can be used in Equation 24 to estimate the emission rate. The resulting expression is

$$C_{i0} = \frac{C_i^* \exp\left(\frac{d_{sc} V_y \tau}{D_i \epsilon}\right)}{\left[1 + \frac{(2.44 \times 10^4) k_{g,i}}{V_y}\right] \left[\exp\left(\frac{d_{sc} V_y \tau}{D_i \epsilon}\right) - 1\right]} \quad (26)$$

The soil-air interface concentration calculated from Equation 26 needs to be substituted in Equation 24 to estimate the emission rate from a landfill.

The terms in Equation 24 can be simplified if the internal gas generation dominates the gas transport processes. The first term in the right hand side of the equation represents the emissions associated with diffusion of the pollutant through the soil pores. The second term represents the convective transport term. Thibodeaux (1981) provided the range of convective velocity of gas being emitted from municipal landfills: 7.29×10^{-4} cm/s to 3.04×10^{-3} cm/s, with an average velocity of 1.63×10^{-3} cm/s for all the landfills cited.

The magnitude of the terms in Equation 24 can be examined using some typical values of experimental data obtained from municipal landfills and radioactive waste sites. At a typical sweep gas velocity of 1.63×10^{-3} cm/s for experimental municipal landfills, the second term (convective term) dominates and the first term can be neglected. On the other hand, for the range of the sweep gas velocity expected in the radioactive waste site (4.44×10^{-7} to 1.27×10^{-5} cm/s), the first term (diffusive term) in Equation 24 dominates. In this latter case, the second term in Equation 24 can be neglected. When this simplification is made, Equation 24 reduces to Equation 16. Hence, Equation 24 can be simplified for use in estimating the emission rate when the internal gas generation is significant. With significant internal generation, Equation 24 can be reduced to

$$E_i = C_i^* V_y A \quad (27)$$

The C_i^* is equivalent to C_{si} in Equation 23 when a waste mixture is disposed of in a landfill and can be evaluated using this equation. The actual concentration of constituent, in the soil space, C_i^* , is a quantity that is not often measured, and as a result, is not expected to always be known. As a conservative approach, the saturated vapor concentration of the constituent, C_{si} , may be used as defined in Equation 22 instead of C_i^* .

2.9 SURFACE IMPOUNDMENTS

EPA's (1988, 1990) model for computing volatilization rates from surface impoundments is implemented in the user-interface (AG-VCASE = 6) of MEPAS 3.n versions. Surface impoundments include ponds (solar evaporation, disposal, or holding), holding tanks, treatment tanks, or any other containment storing or treating of liquid waste. Surface impoundments may hold aqueous type waste or a waste consisting of a mixture of organic substances. The surface impoundment emission model presented in this section is applicable when there is a pool of the liquid containment on the surface of a structure. This model is no longer applicable when volatilization of the contaminant has developed a dry zone (e.g., a layer without any liquid-phase contaminant at the surface). When the dry zone is developed on the entire surface of the contamination, the physical condition relating to volatilization resembles contaminated soil and the emission rate can be estimated with one of the contaminated soil models.

MEPAS uses a model for estimating the emission rates from surface impoundments with undisturbed surfaces because disposal ponds at hazardous waste sites do not normally provide forced agitation on the surface. However, the model provided can be readily adapted to the surface impoundments with turbulent surfaces by simply modifying the values for mass transfer coefficients.

The model for predicting the emission rate is based on the two-resistance theory, which assumes that the resistances to volatilization from the bulk of the liquid to the atmosphere are mainly in the liquid phase and the gas phase as indicated in textbooks and publications (Thibodeaux 1979; Hwang 1982; Mackay and Leinonen 1975). The equation for estimating the emission rate is

$$E_i = K_{L,i} C_{L,i} A \quad (28)$$

where E_i = emission rate of constituent i (g/s)

$K_{L,i}$ = overall mass-transfer coefficient for constituent i expressed in the liquid-phase concentration (cm/s)

$C_{L,i}$ = liquid-phase concentration of constituent i (g/cm³)

A = area of surface impoundment from which emissions occur (cm²).

Equation 28 is a steady-state emission equation and applies when the amount of the constituent i does not change with respect to time. When the amount of the contaminant is finite in the surface impoundment, the emission rate would decrease as the contaminant concentration in the surface impoundment decreases. Equation 28 can be solved as a transient problem for the time-dependent emission rate (Mackay and Leinonen 1975):

$$E_i = K_{L,i} C_{oi} \exp \left[-\frac{K_{L,i}}{d} t \right] A \quad (29)$$

where C_{oi} = initial concentration of constituent i in the surface impoundment (g/cm³)

d = depth of waste liquid in the surface impoundment (cm); the depth can be replaced by V/A where V = volume of waste liquid in the surface impoundment (cm³)

t = time (s).

The average emission rate (\bar{E}_i) over a time period, T seconds, can be obtained by integrating Equation 29 over time:

$$\bar{E}_i = \frac{C_{oi}}{T} \left[1 - \exp \left[-\frac{K_{L,i}}{d} T \right] \right] (A)(d) \quad (30)$$

The overall mass-transfer coefficient can be expressed in either liquid-phase or gas-phase concentration. Equation 28 uses the liquid-phase concentration. When the overall mass-transfer coefficient based on the gas-phase concentration is used in Equation 28, the gas-phase concentration of constitu-

ent i in equilibrium with the liquid phase concentration in the surface impoundment should be used. The overall mass-transfer coefficient relates the volatilization rate from liquid to air. The overall liquid-phase mass transfer coefficient of the constituent can be estimated using a method presented by Hwang (1982):

$$\frac{1}{K_{L,i}} = \frac{1}{k_{L,i}} + \frac{R T}{H k_{g,i}} \left[\frac{C_g}{C_L} \right] \quad (31)$$

where $k_{L,i}$, $k_{g,i}$ = individual liquid-phase and gas-phase mass transfer coefficients, respectively (cm/s)

H = Henry's Law constant ($\text{m}^3 \text{ atm/mole}$) in the database

R = gas constant ($8.2 \times 10^{-5} \text{ m}^3 \text{ atm/mole-}^\circ\text{K}$)

T = temperature ($^\circ\text{K}$).

C_g = molar density of gas (g mole/cm^3); $C_g = 4.1 \times 10^{-5} \text{ g mole/cm}^3$

C_L = molar density of waste liquid (g mole/cm^3); $C_L = 1/18$ for aqueous waste.

In Equation 31, the conversion factor $C_g/C_L = 7.4 \times 10^{-4}$ is necessary in the right-hand side to convert gas-phase units to liquid-phase units.

For constituent i , the individual mass transfer coefficients can be estimated by reference to constituents whose base values are known. Experiments by Owens et al. (1964), Smith et al. (1979), and Thibodeaux (1978) used oxygen as a reference compound for liquid-phase mass transfer and water vapor as a reference for gas-phase mass transfer. Hwang (1982) used equations derived by Cohen et al. (1978), Mackay and Matsugu (1973), Owens et al. (1964), Thibodeaux (1978), and Reinhart (1977) to obtain equations for individual liquid- and gas-phase mass-transfer coefficients for a given constituent.

The equation for computing individual liquid-phase mass-transfer coefficients for natural surfaces is

$$k_{L,i} = \left(\frac{MW_{O_2}}{MW_i} \right)^{0.5} (T/298) k_{L,O_2} \quad (32)$$

where $k_{L,i}$ = individual liquid-phase mass-transfer coefficient (cm/s)

MW_{O_2} = molecular weight of O_2 (32 g/g-mole)

MW_i = molecular weight of constituent i (g/g-mole)

T = annual average air temperature ($^{\circ}K$)

k_{L,O_2} = individual liquid-phase mass transfer coefficient for O_2 at $25^{\circ}C$ (cm/s).

Hwang (1982) evaluated the individual liquid-phase mass-transfer coefficient for oxygen at $25^{\circ}C$ for natural and turbulent surfaces; the coefficient values are 2.2×10^{-3} cm/s for natural surfaces and 2.3 cm/s for turbulent surfaces.

The equation for individual gas-phase mass-transfer coefficients for natural surfaces is

$$k_{g,i} = \left[\left(\frac{MW_{H_2O}}{MW_i} \right)^{0.335} \right] \left[\left(\frac{T}{298} \right)^{1.005} \right] k_{g,H_2O} \quad (33)$$

where $k_{g,i}$ = individual gas-phase mass-transfer coefficient (cm/s)

MW_{H_2O} = molecular weight of H_2O (18 g/g mole)

MW_i = molecular weight of constituent i (g/g mole)

T = annual average air temperature ($^{\circ}K$)

k_{g,H_2O} = individual gas-phase mass-transfer coefficient for H_2O at $25^{\circ}C$ (cm/s).

Hwang (1982) computed individual gas-phase mass-transfer coefficients for water at 25°C of 1.4 cm/s for natural surfaces and 23.2 cm/s for turbulent surfaces.

2.10 SPILL SITES

EPA's (1988, 1990) model for computing volatilization rates from "new spill sites" is implemented in the user-interface (AG-VCASE = 3) of MEPAS 3.n versions. Spills occur when wastes are accidentally released from a containment system. When the spilled material is a liquid waste containing volatile organics, volatilization will occur until the organics are depleted; the volatilization rate may be time-dependent. If the spill occurred on soil, the liquid material will soak into the bulk of the soil while the volatilization process progresses. The duration and the extent of the soaking process will depend upon the characteristics of the soil and the waste. The model used for estimating emission rates from spill sites in MEPAS assumes that a finite but sufficient amount of the original liquid spill remains on the surface of the elements of the soil or pavement. Most emissions are attributable to the liquid above the surface of the spilled object. The equations for estimating emission rates are the same as the equations used for a surface impoundment (Equations 29 and 30). Thus, the emission rate averaged over time, T, from a spill site is

$$\bar{E}_i = \frac{C_{oi}}{T} \left[1 - \exp \left(- \frac{K_{L,i} A}{V} T \right) \right] V \quad (34)$$

where \bar{E}_i = average emission rate over time T (g/s)

$K_{L,i}$ = overall liquid-phase mass-transfer coefficient (cm/s)

C_{oi} = initial concentration of constituent i in the spilled liquid (g/cm³)

V = volume of liquid spilled (cm³)

A = spill area (cm²)

T = emission time over which emission rates are averaged (s).

The overall mass-transfer coefficient to be used in Equation 34 can be obtained from Equations 31, 32, and 33 as described previously.

If a spill is left for some time without cleanup, the spilled volatile materials may no longer be pooled on the surface and the spill model will no longer be appropriate. The spill materials that have not been lost by volatilization (or other processes), will generally be soaked into the underlying surface. The resultant situation will often more closely resemble one of the models for contaminated soil.

2.11 LAND TREATMENT FACILITIES

EPA's (1988, 1990) model for computing volatilization rates from "land treatment facilities" or "old spill sites" is implemented in the user-interface (AG-VCASE = 4) of MEPAS 3.n versions. The use of microbial activity in the upper soil zone to biodegrade oily industrial sludge has been referred to as landfarming or land treatment. Petroleum industries often manage oily residuals by use of the land treatment process. Studies regarding potential air emissions from this process have been reviewed by Thibodeaux and Hwang (1982).

A model developed by Thibodeaux and Hwang (1982) is used for estimating emission rates from land treatment of oily wastes. This model assumes that oily sludge spread on the soil surface forms lumps and films within the soil texture and that these lumps and films dry out slowly as a result of diffusion of vapors through the pores. The loss of contaminant to the air is computed as a function of time, assuming that the soil phase controls the vapor diffusion. Also, the concentration in the contaminant pool is assumed to remain constant until all the liquid-phase contaminant has been lost entirely to the atmosphere. A layering of the contaminant is assumed to occur in the soil consisting of a "dry" surface layer, with low-contaminant concentrations,

located over a "wet" layer with high-contaminant concentrations. The terms wet and dry refer to the presence or absence, respectively, of significant quantities of the contaminant in liquid form. The contaminant is assumed to have pooled in the wet layer and, thus, has uniform concentrations within the layer. In addition to its use for land treatment facilities, this model is also applicable to estimating emissions from soils that contain a pool of waste liquid within the soil.

The emission rate for the land treatment model (also referred to as the old spill model) is computed according to Thibodeaux and Hwang (1982) using

$$E_i = \frac{D C_{si} A}{\left[(d^2) + 2 D t \right]^{0.5}} \quad (35)$$

where E_i = emission rate of the constituent i (g/s)

D = total diffusion from both liquid phase and gas phase (cm^2/s)

C_{si} = liquid-phase concentration of i in the soil (g/cm^3)

A = contaminated surface area (cm^2)

d = depth of the dry layer at time for which analysis begins (cm)

t = time measured from time for which analysis begins (s).

Total diffusion from both liquid phases and gas phases is defined in terms of the flux of the constituent. The constituent first evaporates into voids in the soil and then diffuses into the atmosphere through the dry layer. This value can be estimated by the following equation:

$$D = D_i P_s H_c \quad (36)$$

where D_i = air diffusion coefficient of constituent i (cm^2/s)

P_s = the ratio of air filled to total porosity (Equation 5)
(dimensionless)

H_c = Henry's law constant in concentration form (dimensionless).

Henry's law constant in concentration form, H_c , is defined as the ratio of near-surface air concentration to soil concentration of the constituent. This constant is computed using the following method, given by Lyman et al. (1982):

$$H_c = \frac{H_i}{R T} \quad (37)$$

where H_i = Henry's law constant of constituent i (atm m³/mole)

R = gas constant (8.2 x 10⁻⁵ atm m³/mole-°K)

T = annual average air temperature (°K).

As noted above, this method of estimating the volatilization rate from land-treatment/old spills assumes that a constant pool of concentration of the constituent exists in the soil until all of the constituent has been volatilized to the atmosphere. Based on this assumption, Hwang (1982) provides an equation for computing the dry-out time of a spill as

$$t_d = \frac{(h^2) - (d^2)}{2 D} \quad (38)$$

where t_d = time it takes all of the constituent i to vaporize (s)

h = the depth to the bottom of the contamination (cm)

d = depth of the dry layer (cm)

D = total diffusion coefficient to the atmosphere (cm²/s).

2.12 SURFACE IMPOUNDMENTS WITH SEDIMENT-CONTROLLED EMISSIONS

An alternative model that includes both sediment-to-water transfer and water-to-air transfer processes in surface impoundments is implemented in the user-interface (AG-VCASE = 7) of MEPAS 3.n versions. The surface impoundment formulations given above are not appropriate for cases where the sediment-to-water transfer controls emission rates. Following a method suggested by Thibodeaux^(a) and later documented in Thibodeaux (1989), a model was developed using a set of mass transfer coefficients that control the diffusion of volatile chemicals from the sediment to the water and then from the water to the air. This method is based on experimental work done by Imboden and Emerson (1977) and Thibodeaux and Becker (1982). The combination of this work and the work by Mackay and Leinonen (1975) provides the basis for the MEPAS formulation for computing sediment-controlled gaseous emission rates from a pond or lagoon. The atmospheric emission rates are computed using

$$E_i = \frac{K_{wa} W_a A}{f_{sw} K_d} \quad (39)$$

where E_i = the emission rate of constituent (g/s)

K_{wa} = overall water-side mass-transfer coefficient at the water-air interface (cm/s)

W_a = constituent concentration in sediment (g/g)

A = area of the body of water (cm²)

f_{sw} = sediment-water interface factor (dimensionless)

K_d = partition coefficient between sediment and water concentrations (cm³/g).

(a) Thibodeaux, L. J. 1986. Personal Communication, Chemodynamics 4253 Lecture Notes, Spring 1986, Louisiana State University, Baton Rouge, Louisiana.

Hwang (1991) derives Equation 39 considering the mass-transfer resistances from sediment to water and from water to air. The emission rate is expressed in terms of the constituent concentration in the sediment. The sediment-water interface factor contains coefficients pertinent to resistances in all the phases considered and is given by

$$f_{sw} = \frac{(k_{sw} + K_{wa} + h_s k_r)(k_{ws} + k_{sw}) - (k_{sw})^2}{k_{ws} k_{sw}} \quad (40)$$

where f_{sw} = sediment-water interface factor (dimensionless)

k_{ws} = sediment-side mass-transfer coefficient at the sediment-water interface (cm/s)

k_{sw} = water-side mass-transfer coefficient at the sediment-water interface (cm/s)

h_s = depth of contaminated sediment (cm)

k_r = reaction rate constant in the column of water (s^{-1}).

The sediment-side mass-transfer coefficient can be computed using

$$k_{ws} = \frac{D_w P_a^{1.33}}{h_s} \quad (41)$$

where D_w is the molecular diffusivity in water (cm^2/s) and P_a is the air-filled porosity of the sediment (dimensionless).

The water diffusion coefficient (D_w) can be estimated using the empirical relationship (O'Connor and Muller 1980)

$$D_w = 0.00022 (MW)^{-0.6667} \quad (42)$$

where MW is the molecular weight of the constituent. The coefficient has units associated with it that give values of molecular diffusivity in cm²/s.

The mass-transfer coefficient from sediment to water, k_{sw} , as proposed by Thibodeaux and Becker (1982), is based on a study of the movement of benzoic acid in a wind-water tank. Using the results of this study, they developed the following general formula for computing k_{sw} :

$$k_{sw} = \frac{9.95 \times 10^{-4} CD V_A^2 H_w^{1.25} d_a}{L M^{0.5} d_w} \quad (43)$$

where k_{sw} = water-side mass-transfer coefficient at the sediment-water interface (cm/min)

9.95×10^{-4} = empirical correction factor [(g/mole)^{1/2}min/(cm)^{1.25}]

CD = drag coefficient at the water-air interface (dimensionless)

V_A = wind speed over the water at 10 meters (cm/min)

H_w = average depth of the water column (cm)

d_a = density of the air (g/cm³)

L = average length of the wind fetch (cm)

M = gram molecular weight of the constituent (g/mole)

d_w = density of the water (g/cm³).

The constant 9.95×10^{-4} in Equation 43 is the product of empirical factors and the correction for the molecular weight of benzoic acid. Also, wind and/or thermal forces are assumed to be sufficient for a well-mixed situation to exist in the water.

Hwang (1991) simplified Equation 40 by expanding its terms and comparing the typical values of each term encountered in practical situations. He substituted the simplified Equation 40 into Equation 39 (see Hwang 1991 for the simplification) and presented the following modified equation:

$$E_i = \frac{k_{ws} W_a}{K_d} A \quad (44)$$

Equation 44 shows that, for certain contaminants with a high tendency to partition in the sediment, the sediment-phase controls the release rate of the constituent.

2.13 MASS BUDGET FOR VOLATILES

Source depletion by the loss of volatile constituents to the atmosphere is incorporated in the MEPAS atmospheric component for computing volatilization. The overall source depletion mass budget is discussed in Section 4.10. For all cases, this module assures that the total computed emissions never exceed the inventory of available material. Also for the land treatment/old spill case, no emissions occur after the computed dry-out period.

The total long-term mass losses of volatile materials may be limited by either the emission rates or the total mass of material contained in the landfill, spill, or pond. The atmospheric pathway component computes average lifetime exposures of environmental concentrations based on a 70-year time period. For materials with a relatively rapid volatilization rate (e.g., benzene), a significant reduction in volatile emissions will often occur over the 70-year period, and these computed concentrations will be mainly a function of the total amount of material released rather than initial emission rates (e.g., the values of computed environmental concentrations are a function of the initial site inventory rather than factors controlling the emission rate). At sites where the exact inventory is not known, an upper-limit inventory can be used to avoid an evaluation based on a release of an unreasonably large mass of material. Without input of an estimate of the total mass, MEPAS will assume the same emission rate over the entire 70-year period.

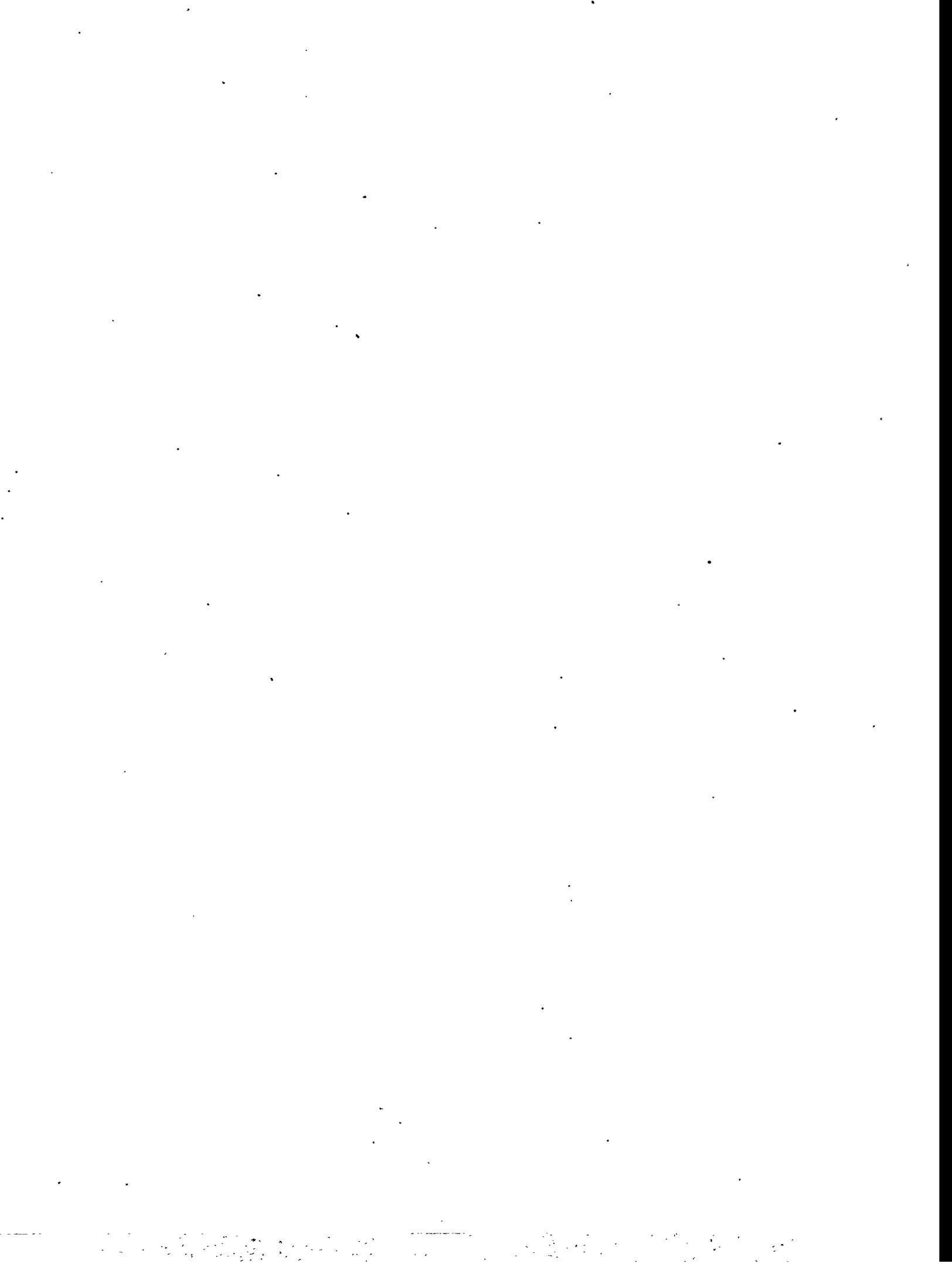
For materials that volatilize relatively slowly (e.g., semivolatiles), the environmental concentrations will normally be a direct function of the emission rates computed with the above volatilization models. However, even for many slowly volatilizing materials, the mass budget limitation can reduce the emission rate significantly over a 70-year time period.

2.14 LIMITATIONS

The volatilization formulations given are simplified estimation procedures that yield approximate release rates based on site and contaminant properties. Although these methods do not account for all the factors that can control these volatile release rates, the estimated release-rates should provide the order-of-magnitude estimates of potential rates required for the MEPAS ranking applications. For site-specific applications a more exact release-rate verification of computed release rates by monitoring data is recommended by the EPA (1988).

The accuracy of the MEPAS volatilization estimate depends directly on how well the problem is characterized. The types, forms, and quantities of chemicals involved need to be defined, along with the physical and chemical properties of the various media.

Because the MEPAS methodology accounts for contaminant loss at the source if the inventory is known, the potential exposures are limited to the amount of material available. However, in cases where the inventory is unknown, the model can release more material than is really associated with the environmental problem. The total releases for cases with undefined inventories should be checked to be certain that such quantities are realistic. Particularly for the more volatile chemicals, an inventory should be defined, even if that inventory is a maximum credible amount for the specific environmental problem.



3.0 INITIAL SOURCE DISPERSION

All releases have initial dilution related to the characteristics of the release. For an area source, the initial dilution is related to the distribution of the release over an area. For a point source, the volume of flow associated with the release controls the initial dilution. Because a sector average model's horizontal dispersion parameter is fixed as a sector width, initial dilution can only be accounted for by increasing the initial vertical dispersion parameter (vertical standard deviation of the distribution of material, σ_z).

3.1 AREA SOURCE

For an area source, such as surface contamination, landfills, and lagoons, the initial vertical dispersion computation depends on whether the receptor is inside or outside the area. For receptors located outside the area, the vertical dispersion parameter is computed based on the distance of the receptor from the center of the area source. This approach assumes the higher concentrations from closer portions of the area will be balanced by lower concentrations from farther portions such that a representative average value will be obtained:

To avoid estimating spuriously high concentrations very near the center of the area, a different approach is used for receptors within the area. For receptors located at the edge, the distance to the center is used. This assumption is consistent with computation outside the area. For receptors located at the center, one-half of the distance from the edge of the area to the center is used^(a). The assumption is that the dilution effect of the area for a receptor at the center can be approximated by point sources located half the distance from the center. For intermediate locations within the area, the distance used to compute the vertical dispersion parameter varies

(a) In practice, the MEPAS dispersion computation does not allow distances less than 100 m.

linearly between the value used at the edge and center of the area as shown in Equation 45.

$$x' = (x + x_a) / 2 \quad (45)$$

where x' = distance for definition of vertical dispersion parameter (m)

x = distance downwind from center of release (m)

x_a = distance from center to edge of area along wind axis (m).

This simplified area dispersion approach assumes that the contribution at a receptor is only from the direction sectors upwind of the receptor's location. Conversely, these direction sectors, centered on the center of area which divide the area into sixteen "pie shaped" areas, only influence concentrations in their direction of influence. This assumption works best when the winds are relatively uniform. For cases where there is a relatively strong wind persistence in one direction, this approach tends to concentrate the influence of that persistence in that direction. The effect will normally be minimal and only occur at distances within, or very close to, the area.

The gross shape of area is accounted for defining the area with an elliptical shape. The radial distances used in the computation are allowed to vary as a function of direction and thus approximate the influence of the area shape on the dispersion. The elliptical shape is limited to N-S and E-W axis.

3.2 POINT SOURCE

For a point source, such as a stack or vent, the initial value of the vertical dispersion parameter is equal to the radius of the release area. The plume from a stack or vent is thus assumed to have an initial size on the order of the stack or vent.

$$\sigma_z' = (\sigma_z^2 + r_s^2)^{0.5} \quad (46)$$

where $\sigma z'$ = resultant vertical dispersion parameter (m)

r_s = radius of release point (m).

3.3 DISCUSSION OF AREA SOURCE AND POINT SOURCE

The different treatment of area and point releases should be kept in mind when deciding which type of source release best fits a situation. The point source assumes an initial dispersion equal to the size of the release, whereby the area source only allows for the effect of a longer travel distance.

The initial source dispersion will only significantly affect the exposures computed at distances very close to the release point (i.e., distances on the same order of magnitude as the dimensions of the release). For most cases, the initial source dispersion will not be a major factor in the determination of overall rankings.



4.0 TRANSPORT, DISPERSION, AND DEPOSITION

Once a contaminant material is airborne, it is transported and dispersed by air movement. The contaminant will be carried by the winds, and the atmospheric contaminant concentration will be reduced by dispersion and deposition processes. The near-surface atmospheric concentrations computed in the transport, dispersion, and deposition module of MEPAS provide the basis for evaluating inhalation exposures.

The relative importance of the atmospheric pathway at various sites is controlled by a combination of topographic and climatological influences. Controlling parameters include the distance and direction from the inactive waste site and the local wind conditions and stability. Because dispersion is a strong function of the downwind distance a contaminant travels, the physical distances between the contaminant site and population centers are of prime importance. The local frequencies of wind occurrence by direction, particularly in areas with topographic channeling of winds, are important in calculating exposure and risk associated with contaminants in the atmospheric pathway. The relative rates of atmospheric dilution between the sites are mainly a function of local wind speeds and dilution (stability) parameters.

As a result of surface-induced mechanical mixing, the local surface roughness influences local dispersion rates. The MEPAS formulation for local dispersion rates accounts for the effect of local surface roughness. All other factors being equal, a site with a smoother surface will have slower dilution rates than a site with a rougher surface.

4.1 ATMOSPHERIC PATHWAY MODEL

A standard straight-line, sector-averaged Gaussian model was selected as the basis of the atmospheric pathway model. Such a model meets the MEPAS objective of assessing long-term, average risk from the various inactive waste sites. This model provides a consistent framework for computing average expo-

tures, and incorporates the major factors that control the initial dilution, transport and dispersion, and deposition of various contaminants.

The sector-averaged atmospheric model is particularly applicable in MEPAS because it allows direct incorporation of long-term site data. The sector-averaged model computes long-term, average exposures by a weighted summation of exposures. These exposures are for a matrix of cases covering the range of combinations of atmospheric stability, wind speed, and wind direction. This model uses climatological data representing average long-term conditions used to define the frequency of occurrence of each case in the computation of an average long-term exposure.

The atmospheric model is not expected to be applicable to all sites. The sector-averaged Gaussian model applies best to sites located on a uniform, flat plane, and is used only as an approximation for sites located on other types of terrain.

Although sites in complex terrain or on a coastline have atmospheric influences that are quite different than sites located on a flat, uniform plane, the use of a straight-line Gaussian model can provide reasonable exposure estimates to the first major terrain feature. As the regional influences become more important at greater distances, the straight-line Gaussian model becomes less accurate.

Information on the MEPAS complex terrain module is included in Section 8.0 of this document. More detailed models for plumes in complex-terrain may be appropriate for use at sites with complex terrain. The MEPAS atmospheric model allows the use of alternative concentration computation codes, if they are found to be essential for a specific site.

Applying the sector-averaged model to sites in complex terrain needs careful attention to ensure that the estimate of risk is reasonable. A wind summary that reflects the transport to the receptors of interest should be selected. For example, if risks to the regional population are needed, then a wind summary typical of the regional transport should be selected. The danger

is that an onsite wind summaries can be dominated by local wind influences and not be appropriate for a regional evaluation.

The Gaussian diffusion equation used for the concentrations of a contaminant in a plume downwind of a continuous point-source release is a standard formulation for atmospheric modeling (see Slade 1968; Bowers et al. 1979):

$$C_k = \frac{Q_k}{2 \pi \sigma_y \sigma_z \bar{u}} \exp \left[-\frac{y^2}{(2 \sigma_y^2)} \right] f(z, H, \sigma_z) \quad (47)$$

where C_k = time-averaged value of concentration for contaminant form k (g/m^3)

Q_k = amount of material released from a point source of a contaminant form k (g/s)

k = index on elemental contaminant form ($k=1, \dots, p$; p = number of forms representing $[p-1]$ ranges of particle sizes, and a gaseous state)

x, y, z = positions in a Cartesian coordinate system that are oriented such that the x-axis is in the direction of the mean horizontal wind vector, the y-axis is cross wind, and the z-axis is vertical height above local ground level (m)

σ_y = standard deviation of the distribution of material in a plume in the y-direction (m)

σ_z = standard deviation of the distribution of material in a plume in the z-direction (m)

\bar{u} = average value wind speed in the x-direction at the height of the plume centerline (m/s)

H = effective height of release over local ground level (m)

$f(z, H, \sigma_z)$ = functional relationship for the vertical variation of plume concentrations (dimensionless).

The function f in Equation 47 has the form of a sum of exponential terms representing the Gaussian dispersion from the actual plume as well from vir-

tual plumes. The use of virtual plumes is a means of accounting for the physical limit on Gaussian vertical dispersion encountered at the ground and at the mixing-height inversion layer. The use of the virtual plumes are important in avoiding a computational loss of mass by dispersion out of the real layer in which the plume exits. The material mathematically "lost" by dispersion of the actual plume through these layers is "recovered" by adding the contributions of virtual plumes. The virtual plumes are thus a means of accounting for plume reflections and multiple reflections at the ground surface and at the mixing height. The form of the function f is based on a discussion by Ramsdell et al. (1983). The vertical exponential term is approximated with a sum of exponentials

$$f(z, H, \sigma_z) \approx \sum_{n=-\infty}^{\infty} \left\{ \exp \left[-\frac{1}{2} \left(\frac{2 n h - H - z}{\sigma_z} \right)^2 \right] + \exp \left[-\frac{1}{2} \left(\frac{2 n h + H - z}{\sigma_z} \right)^2 \right] \right\} \quad (48)$$

where h is the height of the mixing height (m).

As a practical matter, the summation can be truncated after a few terms on either side of zero. In MEPAS, the range of -4 to +4 is sufficient to assure that the computational mass losses are very small at all distances.

The crosswind-integrated concentration from a continuous source is obtained by integrating Equation 46 with respect to the crosswind distance (y) from $-\infty$ to $+\infty$

$$CWI = \frac{Q_k}{\sqrt{2 \pi} \sigma_z \bar{u}} f(z, H, \sigma_z) \quad (49)$$

where CWI = crosswind-integrated concentration (i.e., perpendicular to wind direction) (g/m^2).

The frequency of combinations of wind speeds, wind directions, and diffusion rates can be summarized in terms of a speed, direction, and stability joint frequency table. The average concentration is computed by multiplying the integrated concentration formula (Equation 49) by the frequency of a given set of conditions divided by the width of the sector at the distance of interest. The sector-averaged concentration for one set of wind speed, direction, and stability conditions is given by

$$C_{ijk}(x,z) = Q_k R_k(x) \left(\frac{1}{2\pi} \right)^{1/2} \frac{1}{u_i \sigma_{zj} \left[2\pi \frac{x}{n} \right]} f(z,H,\sigma_{zi}) \quad (50)$$

where $C_{ijk}(x,z)$ = sector-averaged atmospheric concentrations for wind speed, i ; stability condition, j ; and contaminant form, k (g/m^3); for the downwind distance x and height z above local ground level

i = index on wind speed ($i=1, \dots, m$; m = number of wind speed classes)

j = index on stability conditions ($j=1, \dots, n$; n = number of stability conditions)

$R_k(x)$ = deposition and/or decay plume source depletion fraction, which varies as a function of the position x of the plume for contaminant form k (dimensionless)

u_i = wind speed central value for wind speed interval class i (m/s)

σ_{zj} = standard deviation of concentration in vertical for stability class j (m)

n = number of wind direction sectors ($n = 16$) (dimensionless)

$\left[2\pi \frac{x}{n} \right]$ = sector width.

The indexed variables are defined in terms of central values for each atmospheric frequency class (i.e., a set of wind speed, wind direction, and stability conditions). The removal of the contaminant from the atmospheric plume, by various depletion processes, is computed using

$$R_k(x) = r c d w \quad (51)$$

where fractional losses are defined as

r = radioactive decay term (dimensionless)

c = chemical decay term (dimensionless)

d = dry-deposition term (dimensionless)

w = wet-deposition term (dimensionless).

The average air concentration near the earth's surface is input to the inhalation component of the health assessment. The average air concentration, $C(x,z)$ (g/m^3), at ground level ($z = 0$) for a population located at a distance and direction from the waste site is computed as the sum of the concentrations over the i , j , and k indices, given by

$$C(x,z) = \sum_{i=1}^n \sum_{j=1}^m \sum_{k=1}^p [f_{ij} C_{ijk}(x,z)] \quad (52)$$

where f_{ij} = climatological fractional frequency of occurrence of the wind speed (i) and stability class (j) conditions within the specified direction (dimensionless).

The table of frequencies of occurrence of the f_{ij} values is referred to as a joint-frequency summary. These data are available as summaries referred to as "STAR data" from the National Climatic Data Center, Asheville, North Carolina.

The local surface roughness is characterized by a surface roughness length. Table 4.1 (and Figure 2.1) show examples of the magnitude of this parameter for various surface covers. The surface roughness lengths in the region surrounding the release are used to account directly for local influences in both dispersion and dry-deposition computations.

The central wind speed, u_1 , in a wind-speed category is not necessarily applicable to the movement of an atmospheric plume in a region of interest. The wind speed needs to be adjusted for differences in height and local surface roughness. The atmospheric component of MEPAS uses relationships from atmospheric surface layer similarity theory given by Paulson (1970), Businger et al. (1971), and Hanna et al. (1982) to compute an equivalent central wind speed at plume height for each wind speed category. To provide a height adjustment of the wind speed as a continuous function of the local surface roughness, these relationships are used in preference to less general power-law approximations (Irwin et al. 1985).

For neutral atmospheric conditions, the following expression is used to calculate the wind variation with height (Paulson 1970):

TABLE 4.1. Typical Surface Roughness Lengths

<u>Surfaces</u>	<u>Roughness Length (cm)</u>
Snow, sea, desert	0.005 - 0.03
Lawn	0.1
Grass (5 cm)	1 - 2
Grass (tall)	4 - 9
Mature root crops	14
Low forest	50
High forest	100
Urban area	>100

$$\bar{u} = \frac{u_*}{0.4} \ln \left(\frac{z}{z_o} \right) \quad (53)$$

For unstable atmospheric conditions, the following expression is used to calculate the wind variation with height (Paulson 1970):

$$\bar{u} = \frac{u_*}{0.4} \left[\ln \left(\frac{z}{z_o} \right) - 2 \ln \left[\frac{1}{2} \left(1 + \frac{1}{\phi_m} \right) \right] - \ln \left[\frac{1}{2} \left(1 + \frac{1}{\phi_m^2} \right) \right] + 2 \tan \left(\frac{1}{\phi_m} \right) - \frac{\pi}{2} \right] \quad (54)$$

where \bar{u} = average wind speed (m/s)

u_* = friction velocity (m/s)

z = height over land/water surface (m)

z_o = roughness length of surface (m)

ϕ_m = wind-gradient parameter (dimensionless).

In MEPAS, the sum of the last three terms is approximated using a literature-derived central value of 0.458.

For stable conditions, the following expression is used to calculate the wind variation with height (Hanna et al. 1982):

$$\bar{u} = \frac{u_*}{0.4} \left[\ln \left(\frac{z}{z_o} \right) + 5 \frac{z}{L} \right] \quad (55)$$

where L is the Monin-Obukhov length (m), a scaling length of atmospheric turbulence. Equations 54 and 55 are integrated forms of relationships derived from field studies by Businger et al. (1971).

To use Equations 52, 53, and 54 for determining the wind variation with height, the roughness length, friction velocity, and Monin-Obukhov length must be known or calculated.

Empirical relationships are used in the MEPAS atmospheric model to estimate the friction velocity (u_*) over water surfaces. These friction velocity relationships were taken from drag coefficient relationships reported in Large and Pond (1981) by substituting for the friction velocity using $C_D = u_*^2/u_x^2$:

$$\begin{aligned} u_* &= 0.0346 u_x && \text{for } 4 \leq u_x < 11 \text{ m/s} \\ u_* &= 0.0316 u_x (0.49 + 0.065 u_x)^{1/2} && \text{for } 11 < u_x \leq 25 \text{ m/s} \end{aligned} \quad (56)$$

where u_x = wind speed at the 10-m height.

The roughness length is an input parameter for overland surfaces. Charnock's relationship for the roughness length (z_o), as described by Joffre (1985), is used for overwater surfaces:

$$z_o = \frac{m u_*^2}{g} \quad (57)$$

where g = acceleration of gravity (m/s^2)

m = coefficient (= 0.0144; recommended by Garratt [1977]).

The Monin-Obukhov length is a function of atmospheric stability and is related to the Pasquill stability class and roughness length using the relationship of Golder (1972).

Using the approach of computing appropriate wind speeds for the underlying surface allows the wind speeds to vary as a function of distance downwind of the release. The plume speed is computed at a height of the approximate vertical center of mass of the plume at each downwind distance.

This speed is used to compute a travel time for each computation interval. The total travel time divided by the distance traveled defines an average plume speed for use in Equation 50.

4.2 TOTAL DEPOSITION

The deposition to surfaces can occur as the result of both wet- or dry-removal processes. Wet removal is caused by the scavenging and deposition of the contaminant by precipitation or cloud droplets. Dry deposition is the direct deposition of the airborne contaminant onto a surface by processes such as impaction, sorption, and gravitational settling. The total deposition for wet and dry processes provides surface contaminant levels for the overland transport pathway and also provides the basis for evaluating ingestion exposures from the atmospheric pathway.

The total deposition to the surface is input to the exposure component of the MEPAS model. The total deposition at a specified location is computed as the sum of the wet- and dry-deposition fluxes to the surface:

$$T(x,z) = \sum_{i=1}^n \sum_{j=1}^m \sum_{k=1}^p [f_{ij} D_{ijk}(x,z) + g' W_{ijk}(x,z)] \quad (58)$$

where $T(x,z)$ = total surface concentration (g/m^2)

$D_{ijk}(x,z)$ = dry-deposition flux (g/m^2)

$W_{ijk}(x,z)$ = wet-deposition flux (g/m^2) for wind speed (i), stability class (j), and contaminant form (k)

g' = climatologic fractional frequency of occurrence of the indexed precipitation conditions within the specific direction (dimensionless).

The formulations of the dry and wet deposition models are discussed below in Sections 4.7 and 4.8, respectively.

4.3 DISPERSION COEFFICIENTS

The MEPAS atmospheric pathway component uses six classes of atmospheric stability to characterize the dispersion rates. The atmospheric stability classes are designated by the letters A to F (Slade 1968) and are commonly referred to as the Pasquill Stability Categories (Pasquill and Smith 1983). The classes A, B, and C stand for very unstable, unstable, and slightly unstable conditions, respectively; D stands for a neutral condition; and E and F stand for stable and very stable conditions, respectively. Dispersion varies from being fastest for very unstable conditions to being slowest for very stable conditions.

The Pasquill dispersion curves used in the atmospheric component of MEPAS are computed as a function of elapsed plume travel time. The conversion from the distance dependence to the time dependence is based on equivalent wind speeds. The Pasquill curves are applied as a function of time for the conditions for which the curves were originally developed. Following Hasse and Weber (1985), the Pasquill dispersion curves are assumed to apply over rural English countryside ($z_0 = 10$ cm). Equations 51 and 52 are used to compute wind speeds. The plume travel time is computed as the sum of travel times over various surfaces, thus allowing for local wind shear effects in the dispersion computation.

The MEPAS formulation that accounts for local roughness influences is particularly important in cases where the wind data are from a location with a quite different surface roughness than the site. The MEPAS formulation also accounts for changes in surface roughness in the region:

In terms of the computed dilution rate in the air, the roughness influences on dispersion rates and wind speed tend to cancel each other. As a result of surface-induced mechanical mixing, the local surface roughness influences local dispersion rates and the wind speed profile. At a given distance from the source, a site with a smoother surface will have smaller dispersion rates and larger near-surface wind speeds than a site with a

rougher surface. The equation for computing sector-average air concentrations (Equation 47) contains the product of the vertical dispersion rate and the wind speed. All other factors being equal, these two local surface influences almost exactly cancel each other. The result is that the computed dilution at a potential receptor location does not vary with the surface roughness.

Even though the dilution does not vary with surface roughness, the computed concentrations and deposition rates will vary with surface roughness. The roughness-induced changes in dispersion rate and wind speed directly change the estimated deposition rates. Deposition rates indirectly change computed air concentrations by the plume depletion rate.

4.4 CALM AND MISSING WIND CONDITIONS

The MEPAS atmospheric component uses six classes of atmospheric stability to characterize the dispersion rates. The atmospheric stability classes are designated by the letters A to F (Slade 1968) and are commonly referred to as the Pasquill Stability Categories (Pasquill and Smith 1983).

In the characterization of frequency of winds in each of these stability classes, often some fraction of the reported cases are for calm or zero wind speed conditions. Since the formulations for the climatological atmospheric component require a non-zero wind speed, a method was adopted for handling the reported calm conditions based on assigning these conditions a low, non-zero wind speed in a manner that reflects the occurrences of winds with low wind speeds. This procedure is appropriate because calm conditions are more correctly defined as conditions when the winds are less than the starting speed of the anemometer--the atmosphere is very seldom really calm with no air movements.

The occurrences of calm conditions in each stability class are distributed in a special wind speed class. The relative frequencies of occurrence of winds in the lowest wind speed class are used to distribute calms as a function of direction. If the lowest wind speed class has no entries, then

the calms are distributed equally over the 16 direction sectors. Calm conditions are modeled with a wind speed of 0.5 m/s.

The input table of dispersion conditions is normalized to represent all conditions. That is, missing conditions are distributed according to the input frequencies of occurrence.

4.5 RADIOACTIVE DECAY

Radioactive materials with short half-lives may undergo significant radioactive decay while still airborne. The radioactive decay plume depletion term (r) (see Equation 51) is based on the following expression:

$$r = \exp\left[-\frac{\lambda x}{u_i}\right] \quad (59)$$

where λ = first-order decay coefficient (s^{-1})

x = downwind distance (m).

The term u_i is as defined for Equation 50. EPA (1979) relates the decay coefficient to the contaminant half-life $T_{p_{1/2}}$ (s) using

$$\lambda = \frac{0.693}{T_{p_{1/2}}} \quad (60)$$

4.6 CHEMICAL REACTIONS

For computation of long-term effects, the near-field reactions during airborne transport are not expected to be important for most materials. However, in special cases, the resultant plume depletion fraction is computed using Equation 61.

Chemical reactions that are fast enough to significantly change the airborne concentrations within the plume may be accounted for using a first-order degradation coefficient (λ). The fraction of the contaminant lost to degradation can be expressed as follows (EPA 1979):

$$c = \exp\left[-\lambda \frac{x}{u_1}\right] \quad (61)$$

where c = chemical degradation term in Equation 51.

4.7 DRY DEPOSITION

The dry deposition rate is computed using a total resistance (R_{ijk}) as shown in Equation 63. The total resistance, the inverse of the deposition velocity, is computed at each point as the sum of atmospheric and surface resistances:

$$R_{ijk} = R_{a_{ijk}} + R_{s_{ijk}} \quad (62)$$

where $R_{a_{ijk}}$ = atmospheric resistance (s/m)

$R_{s_{ijk}}$ = surface resistance (s/m) for wind speed (i), stability class (j), and contaminant (k).

The atmospheric resistance represents the resistance for the transfer of a contaminant in the atmospheric layer to the ground surface. The atmospheric resistance varies with the wind speed, stability, and upwind surface roughness using micrometeorological relationships (Paulson 1970; Businger et al. 1971; Golder 1972). The surface resistance is a function of the surface roughness and the properties of the materials. For particulate matter, the gravitational term is included in the empirical curves used to define the resistances (Sehmel and Hodgson 1978).

Dry deposition is based on the computed near-surface air concentrations given in Equation 48 using

$$D_{ijk}(x,z) = \frac{C_{ijk}(x,z) t'}{R_{ijk}} \quad (63)$$

where R_{ijk} = dry-deposition resistance (s/m) for wind speed (i), stability class (j), and contaminant (k)

t' = time period for deposition (s).

A mass budget approach is used to compute the net Gaussian plume source depletion fractions (i.e., parameter d in Equation 49) for dry deposition. Although these removal rates are applied as a source depletion model (see Equation 48) such as the one given in Slade (1968), the surface depletion effects documented by Horst (1984) are accounted for in the MEPAS dry deposition model by the atmospheric resistances. The approach computes deposition resistances for each wind speed/stability class over a layer that is deep enough so that corrections for near-surface concentration depletion are unnecessary. The thickness of this layer is assumed to be 10 m. The computation of the atmospheric resistance term is based on assuming empirical shapes of micrometeorological profiles. The atmospheric resistance varies with stability, wind speed, and local surface roughness.

4.8 WET DEPOSITION

The detailed calculation of the scavenging of contaminants from individual plumes requires a complex model with a number of inputs that are difficult to define. The MEPAS calculation of climatological scavenging of contaminants is accomplished using a simpler approach (Slinn 1976). The climatological calculation used in MEPAS provides estimates of wet deposition rates. This computation accounts for the major factors changing the wet deposition for the various combinations of releases and receptors between sites.

The wet deposition involves integration of the scavenged material over height. Hanna et al. (1982) expresses the integrated wet flux (F_{wet}) for rain falling completely through a Gaussian plume as

$$F_{\text{wet}} = \frac{\Lambda Q_k}{\sqrt{2\pi} \sigma_{y_j} u_i} \quad (64)$$

where F_{wet} = scavenged flux ($\text{g}/\text{m}^2\text{-s}$)
 Λ = scavenging coefficient (1/s).

Equation 64, converted to a sector-averaged form for the total deposition, is expressed as

$$W_{ijk}(x,z) = \frac{8 \Lambda Q_k R_k(x) t'}{u_i \pi x} \quad (65)$$

This relationship for $W_{isk}(x,z)$ is input for Equation 58. The contaminant removal term, R_k , is determined from Equation 51. The scavenging coefficient for a specified volume of a plume is defined as the airborne contaminant removal by precipitation scavenging. Hanna et al. (1982) point out that the scavenging coefficient varies with the rainfall type and rate, saturation conditions, and contaminant characteristics. The MEPAS implementation of this model assumes a neutral stability for all precipitation conditions. The wet deposition plume depletion term (w in Equation 51) is obtained using

$$w = \exp\left[-\frac{\Lambda x}{u_i}\right] \quad (66)$$

Hanna et al. (1982) points out that this method applies to monodisperse particles or to highly reactive gases that are irreversibly scavenged. As such this method is limited to providing upper-limit estimates that maximize the near-source wet-removal rates.

4.9 DEPOSITION CLASSES

The dry and wet deposition rates are computed as described above. A mass budget approach is used to compute the deposition of net Gaussian plume source depletion fractions as a function of distance from the release.

The implementation of removal rates is accomplished in MEPAS using seven deposition classes which represent the constituent properties shown in Table 4.1. The air concentration and deposition patterns are computed for each of these classes based on a unit emission rate. Depending on the properties of a constituent, each constituent is assigned to a deposition class. Then the air concentration and deposition patterns for each constituent are computed using the appropriate normalized concentration patterns and the constituent emission rate.

TABLE 4.2. Definition of Deposition Classes

Deposition Class	Class of Constituent
1	particles with average radius = 7.5 μ
2	particles with average radius = 3.0 μ
3	particles with average radius = 0.3 μ
4	gas with moderate surface resistance (s/cm)
5	nondepositing gas ^(a)
6	gas emission that deposits as a Class 3 particle
7	gas with fast deposition rate (zero surface resistance)

(a) In terms of atmospheric plume depletion computation. Constituent deposition will be computed in exposure computation.

In the MEPAS user interface the deposition classes are allocated in the following manner.

The constituent database contains a "default" entry for the deposition class for each constituent. If the material is released in a particulate form, this value is 1 indicating that one of the first three classes are appropriate. The MEPAS user interface assumes that Class 1 is most appropriate for area releases of suspended soil materials and that Class 3 is most appropriate for point releases (stack and vent releases). Class 2 is not currently available through the MEPAS user interface. If the material is released in a gaseous form, then the constituent database contains the most appropriate value from Classes 4, 5, 6, and 7.

4.10 SOURCE MASS BUDGET

The emission of a constituent will deplete the inventory of that constituent at the site. With one exception, the depletion of the mass by a gaseous emission in the inventory of an area source is assumed to proportionally reduce the emission rate. The exception is for the case of a landfill treatment/old spill volatilization computation where a constant emission rate is assumed with a linear reduction in the inventory. The depletion of mass for particulate emissions also does not change the emission rate.

For sites where the inventory is known, or can be estimated, the proportional depletion is computed using

$$f_m = e^{-t/h} \quad (67)$$

where f_m = mass emission depletion fraction

t = elapsed time (s)

H = mass removal half-life (s).

In the current MEPAS user interface implementation, the default is to assume that source depletion occurs for all gaseous and particulate constituents in an area source case for which inventories are input. The investigator has the option of defining an average emission rate for a 70-year period with no inventory, or an initial emission rate with the inventory. The former requires that the investigator externally account for mass depletion, and the latter allows use of MEPAS formulations to account for the source depletion.

4.11 PLUME RISE

Plume rise formulations given by Briggs (1969, 1971, 1973, 1975) and reported in Petersen et al. (1984) are used in the MEPAS atmospheric model. The plume rise equations are based on the assumption that plume rise depends on the inverse of the mean wind speed and is directly proportional to the two-thirds power of the downwind distance from the source. Different equations are used for different atmospheric stabilities.

The plume rise equations used for unstable and stable atmospheric conditions are summarized below. For additional details of the plume rise formulation, the reader is referred to the detailed description of the plume rise formulations by Petersen et al. (1984).

4.11.1 Unstable and Neutral Atmospheric Conditions

The plume rise relationships are as follows:

$$x_f = 3.5 x^* \quad (68)$$

where x_f = downwind distance of final plume rise (m)

x^* = distance at which atmospheric turbulence begins to dominate entrainment.

The value of x^* is computed from

$$x^* = 14 F^{5/8} \quad \text{for } F < 55 \frac{\text{m}^4}{\text{s}^3} \quad (69)$$

or

$$x^* = 34 F^{2/5} \quad \text{for } F \geq 55 \frac{\text{m}^4}{\text{s}^3} \quad (70)$$

where F is the buoyancy flux parameter (m^4/s^3). The final plume rise is given by

$$H = h' + \frac{1.6 F^{1/3} (3.5 x^*)^{2/3}}{u_h} \quad (71)$$

where H = effective height of plume (m)

h' = stack height above sea level adjusted for stack downwash (m)

u_h = wind speed at top of stack (m/s).

4.11.2 Stable Atmospheric Conditions

The relationships for distance expressed as a function of stability parameter are

$$x_f = 0.0020715 u_h s^{-1/2} \quad (72)$$

where s = stability parameter (1/s).

The plume rise height for windy conditions is given by

$$H = \bar{h}' + 2.6 \left[\frac{F}{(u_h s)} \right]^{1/3} \quad (73)$$

or for near-calm conditions

$$H = \bar{h}' + 4 F^{1/4} s^{-3/8} \quad (74)$$

The lower value of H computed from these two equations is used as the final plume rise.



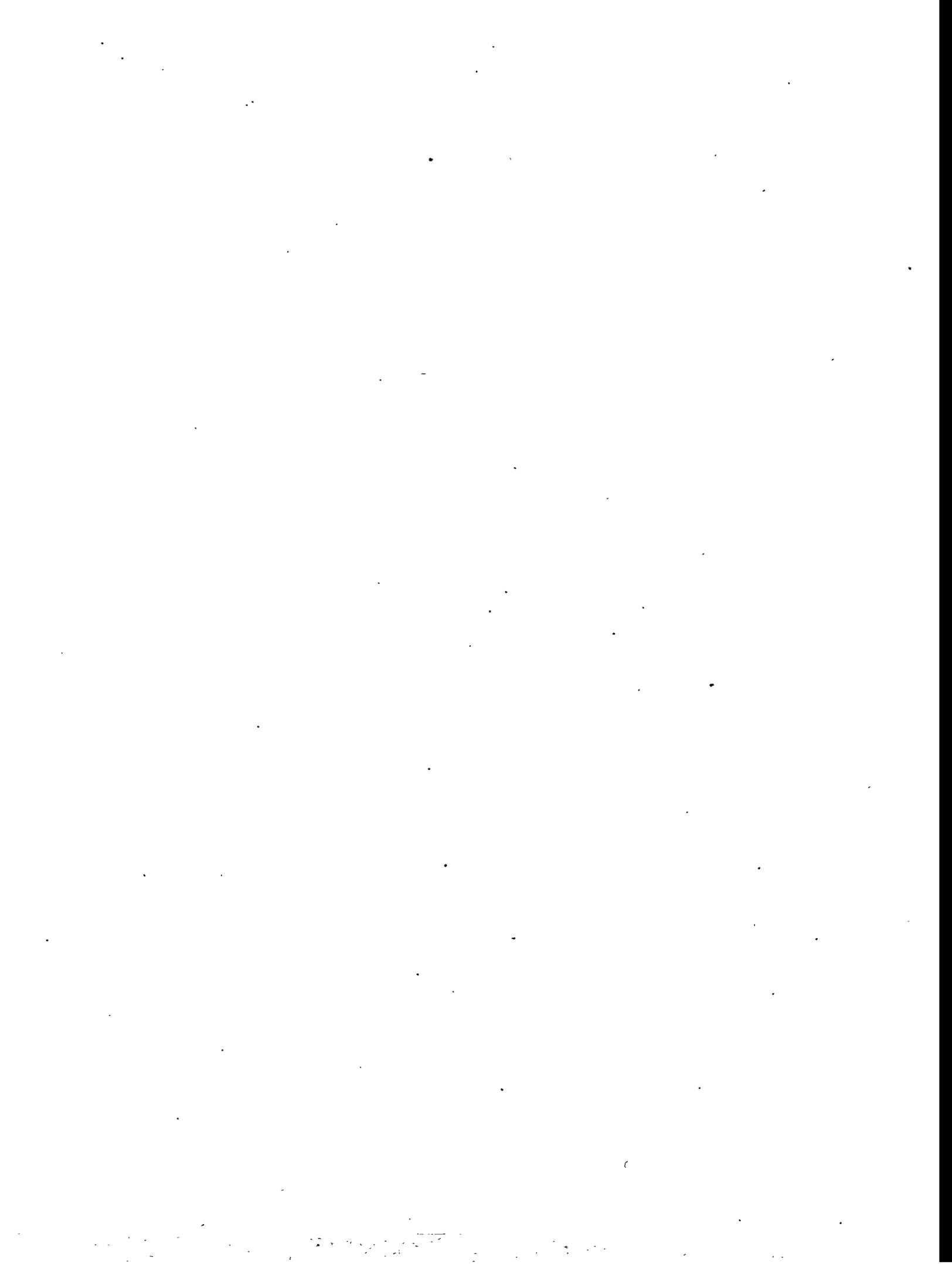
5.0 AIR AS SOURCE

The air-as-source component is an input option that allows the investigator to input a uniform regional air concentration of a contaminant. The exposure pathways are computed based on having the same concentrations and deposition rate everywhere over the region. That is,

$$C(x,\theta) = C_i \quad (75)$$

where $C(x,\theta)$ is the air concentration at any arbitrary distance, x , and direction, θ (degrees); and C_i is the input value for ambient air concentrations (g/m^3).

Applications for the air-as-source component are mainly for evaluation of background concentrations from sources of distant and/or poorly defined origin. The air-as-source component may also be used to approximately evaluate impacts from a disperse regional source term such as roadways.



6.0 INDOOR AIR CONCENTRATION

An indoor air concentration component was added to allow evaluations of long-term climatological exposures in residences.

The residence structure is assumed to be within one of the directional computation sectors used in the implement of the sector average Gaussian dispersion model. Two influences of the structure on indoor concentrations are considered: indoor filtration/deposition and enhanced dispersion. The use of a sector average dispersion model means that the lateral dispersion (i.e., width of the building) will not be important in the concentration computation. If plume has not sufficiently dispersed vertically to envelop the structure, enhanced indoor vertical mixing can reduce the indoor concentrations compared to outdoor concentrations. The filtration/deposition process which is a function of contaminant properties will apply in all cases. The indoor concentration is computed using

$$C' = C_{ijk}(x, z)' * (1 - F_r) \quad (76)$$

where C' = indoor concentration (g/m^3)

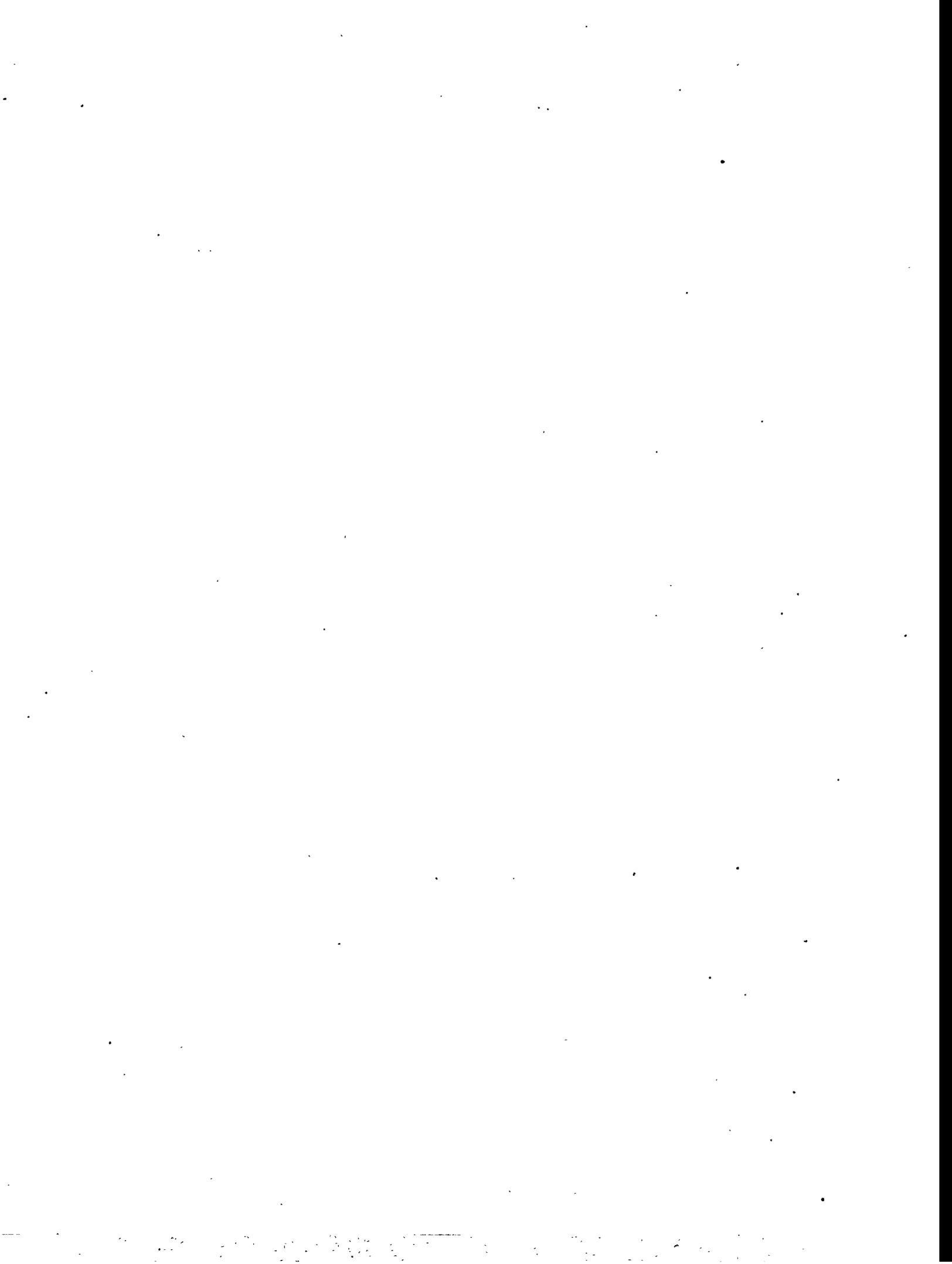
$C_{ijk}(x, z)'$ = outdoor air concentration with σ_z minimum of h_b (g/m^3)

F_r = filtration efficiency fraction (dimensionless)

h_b = interior height of building (m).

The MEPAS model default values for F_r are 0.9, 0.5, 0.10, 0.50, 0.0, 0.10, and 0.90 for deposition classes 1, 2, 3, 4, 5, 6, and 7, respectively. The default value for h_b is 2.44 m.

The average indoor concentration is computed in the same manner as the outdoor concentration by summing the contributions for all ambient conditions. Although the options for indoor concentrations are not incorporated in the current MEPAS user interface, indoor concentrations computed based on default values are computed and available in intermediate output files.



7.0 DISPERSE REGIONAL IMPACT

For some applications, the source of the contaminant emissions may be many release points spread over the region. The emissions from home heating furnaces are an example of such a source. A detailed evaluation of the thousands of release points is, at best, a difficult task.

A component was developed for consideration of cases with a disperse regional source term. This component operates in a three-step process. First, the concentration and deposition patterns for a single typical release point are defined. Second, scaled patterns from the first step are superimposed to define the maximum cumulative impact of sources over the region on a typical single receptor located in the center of the region. Third, the air-as-source option described above is used to evaluate impacts over the region.

This analysis requires definition of the density and intensity of sources in annular segments as a function of distance and direction from the facility. The component allows use of a correlation with population to define the density of sources. The single typical release computation results define air and surface concentrations as a function of distance and direction. These concentrations can be used to compute approximate downwind concentrations from multiple sources within an area using

$$\begin{aligned} C &= C_f C_d A_d \\ D &= D_f C_d A_d \end{aligned} \tag{77}$$

where C = air concentration (g/m^3)

D = surface deposition (g/m^2)

C_f = air concentration for unit source (g/m^3)

D_f = surface concentration for unit source (g/m^2)

C_d = density of unit sources in area (number/m²)

A_d = area (m²).

This formulation assumes the sources all have the same, or nearly the same, release characteristics as the typical unit release. Then by adding the contributions from each of the annular segment areas surrounding the central receptor point, the cumulative exposure of the disperse sources is computed:

$$\begin{aligned} C_c &= \sum_{dir=1,16} \sum_{dis=1,20} C \\ D_c &= \sum_{dir=1,16} \sum_{dis=1,20} D \end{aligned} \tag{78}$$

where C_c = cumulative air concentration (g/m³)

D_c = cumulative soil deposition (g/m²)

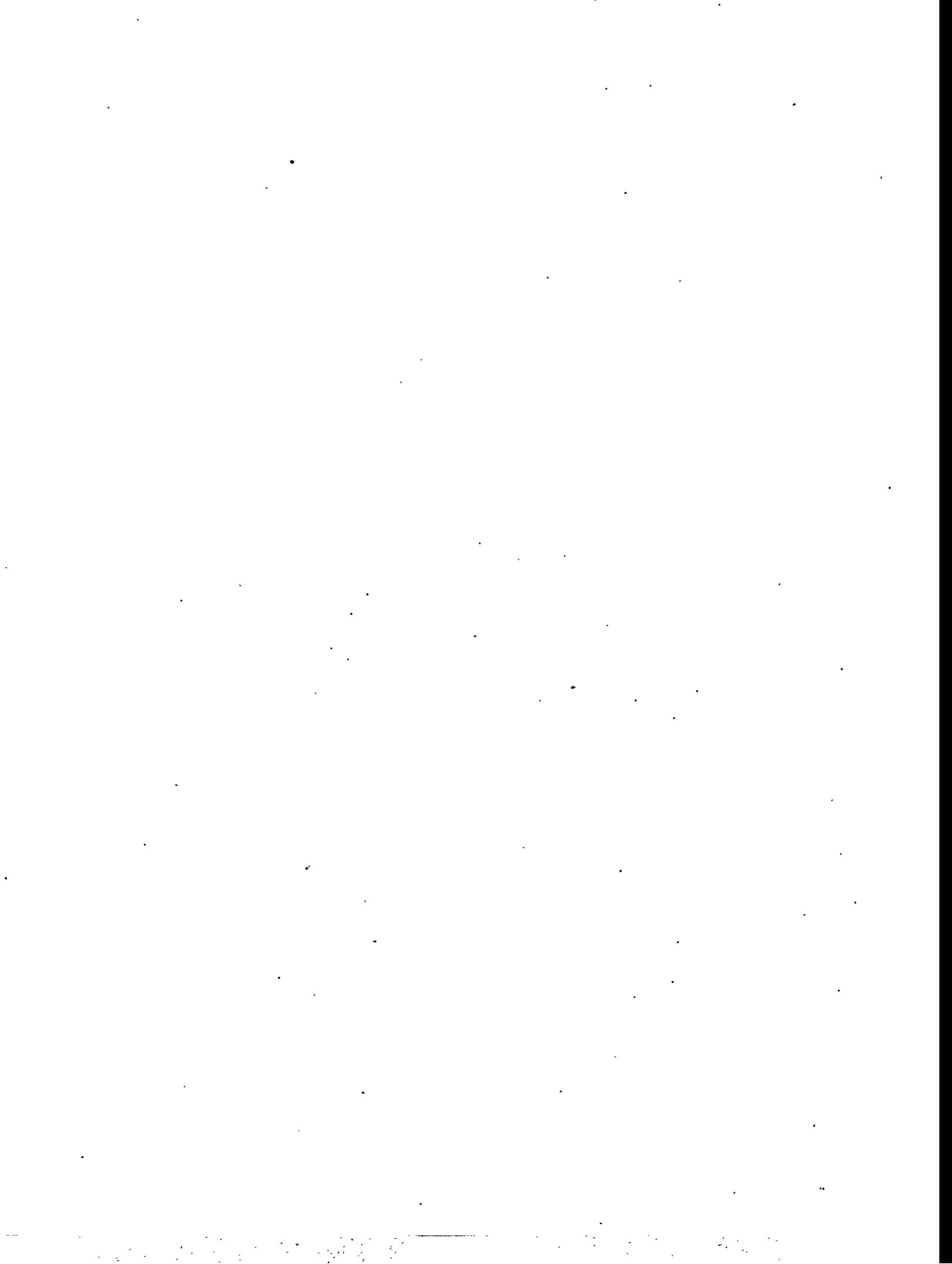
dis = distance from the center of the area (m)

dir = direction from the center of the area (m).

Then C_c and D_c are used as air-as-source inputs to evaluate impacts over the region.

The disperse regional source term provides a convenient method of handling cases with numerous release points over the region. Although the approach of using densities of release points greatly simplifies the data requirements, it also limits the resolution of applications. This approach will work best for many similar sources spread relatively uniformly over the region in question. The approach should not be used for cases with either a limited number of sources or a non-uniform regional distribution of sources. The key to deciding if an application is appropriate is to decide if the sources are numerous and disperse enough that a uniform concentration pattern can be used to evaluate exposures. The disperse regional source-term com-

ponent has not been incorporated into the MEPAS user interface and currently is run only for special applications.



8.0 COMPLEX TERRAIN COMPONENT

MEPAS is designed to consider environmental emissions of potentially hazardous materials. When such materials are released to the atmosphere at sites surrounded by flat uniform terrain, the atmospheric MEPAS component can be used to compute potential airborne concentrations and surface deposition rates. For sites with complex nonuniform surrounding terrain, additional enhancements have been added that allow for the influence of such terrain features. This section presents mathematical formulations and assumptions adopted within MEPAS for complex terrain applications.

The complex terrain components described below are only approximations of the major consequences of local terrain effects on atmospheric transport and dispersion. In his overview of processes in complex terrain, Orgill (1981) describes specific terrain-induced airflow phenomena over various types of landforms along with the technical difficulty of modeling these phenomena. Case-specific models of flow in complex terrain tend to be computer-intensive models. However, such models were not considered appropriate for generating the long-term average concentration patterns needed in MEPAS.

8.1 BACKGROUND

The trajectory and diffusion of an atmospheric plume are known to be influenced by complex terrain. A number of models have been developed to emulate special processes in complex terrain (i.e., Burt 1977; Hovind et al. 1979; Strimaitis et al. 1983; Allwine and Whiteman 1988; Bader and Whiteman 1989). The effects of the underlying surfaces can modify the transport, dispersion, and deposition processes. Areas with high ground-level concentrations can occur as the result of two different complex terrain effects. First, under moderate or high wind conditions, an elevated plume may impinge on local topographical features resulting in localized high-level concentrations. Second, under low wind or stable atmospheric conditions, a channeling of releases in a single direction can maximize ground-level concentrations.

MEPAS accounts for the effects of underlying surfaces on the vertical wind structure and the deposition rate of airborne pollutants onto these surfaces. These formulations are designed to improve the computations of climatological transport, dispersion, and deposition for a given site by using site-specific input data.

A straight-line Gaussian atmospheric model, which assumes the plume trajectories are in straight lines from a central release point, cannot account for the processes in complex terrain where the winds tend to follow local topographical features (valleys, gorges, slopes, etc.). A modified model has been developed that incorporates the major influences of local channeling for wind channeling in the immediate vicinity of the release.

An elevated release which is lower than surrounding terrain may intersect local topographical features. Studies have shown that the tendency for the plume to intersect a hill is a function of the ambient meteorological conditions. The techniques described by Hanna et al. (1982) for accounting for topographical interactions in complex terrain have been adapted for application in the MEPAS climatological dispersion component. The formulations given below account for the tendency for winds to intersect or flow over terrain features depending on ambient atmospheric conditions.

8.2 PLUME INTERSECTION WITH TOPOGRAPHICAL FEATURES

The algorithms for plume intersections with local topography closely follow techniques suggested by Hanna et al. (1982). For unstable and neutral conditions, the plume height is reduced by up to 50% based on the height of local terrain. That is

$$\begin{aligned} H' &= H - H_t && \text{for } H_t < H/2 \\ H' &= H/2 && \text{for } H_t > H/2 \end{aligned} \tag{79}$$

where H' = plume height over local terrain (m)

H = plume height based on elevation of release point (m)

H_t = height of local terrain over elevation of release point (m).

For stable conditions, the plume is assumed to impinge directly on local topographical features and subsequently follow the features. The plume height is computed as

$$\begin{aligned} H' &= H - H_t && \text{for } H_t < H \\ H' &= 0 && \text{for } H_t > H \end{aligned} \tag{80}$$

with an additional restriction that the plume height is never allowed to increase as a function of distance as a result of terrain effects. If the terrain would result in a plume rise increase at a given distance, then the plume is maintained at the plume rise computed for the previous distance.

8.3 LOCAL CLIMATOLOGICAL PLUME CHANNELING

The importance of local circulations on exposures is a function of the size of the plume relative to the scale of the local circulations. Initially the plume is smaller than the local circulation, and the entire plume trajectory will be determined by the local circulation. As the plume travels, the dimensions of the plume increase and the local circulations become progressively less important in computing exposures.

The trajectories of ground-level releases will be affected by local wind channeling. The trajectories of elevated releases will be affected except in cases where the height of the plume is not within the local circulation.

Depending on the local topographical conditions, the trajectories in the immediate vicinity of the release can be important for the computation of both maximum individual and total exposures. The consideration of local channeling is most important in cases where the exposures to people will be significantly

changed. In the absence of local populations, the local channeling may still be needed if predicted air concentrations are being evaluated.

The frequency of occurrence of winds in the direction of the downslope flow from the release point are assumed to be enhanced by the local channeling effects. Downslope winds driven by nocturnal cooling are assumed to occur mainly under stable atmospheric conditions. The winds are progressively coupled back into the regional winds either when the plume has dispersed to the height of the channel or at the end of the channel.

Upslope winds are driven by the tendency of warmer air to rise, whereby downslope winds are driven by the tendency of cooler air to fall. The natural warming and cooling processes at the surface make the overlying air layer unstable and stable, respectively. Hence the upslope winds tend to have fast dispersion rates and downwind winds tend to have slow dispersion rates.

The MEPAS atmospheric component computes total exposure to people in the region surrounding the release. This total exposure is the sum of a matrix of stable, neutral, and unstable conditions. The MEPAS local channeling module accounts for the channeling under the slow dispersion (stable) conditions. For neutral and unstable conditions, no special formulations are used to account for channeling.

All stable conditions (Pasquill categories E, F, and G) are assumed to be nocturnal drainage conditions for the site. The winds for these stable conditions are assumed to flow in the downslope direction with a nominal initial wind speed of 2.0 m/s at 1-m height, which is consistent with typical wind observations in complex terrain (Orgill 1981).

Within the channel, the air concentrations for stable conditions are computed using

$$C = Q/\sigma_z Y/u \quad (81)$$

where Q = emission rate (g/s)

C = air concentration (g/m^3)

Y = the horizontal dispersion width (m)

u = wind velocity (m/s).

The other term in the equation, σ_z , is as defined in Equation 45. Once the plume becomes as deep as the channel, it is assumed to start dispersing out of the channel. The plume is approximated using a sector average "release" of material with initial dispersion equal to the depth of the channel. An initial width equal to the channel width is used. The coordinates of this "release" are centered at the point where the vertical dispersion parameter, σ_z , has increased to the depth of the channel.

Figure 8.1 illustrates the channeling model for the case where the plume reaches the end of the channel before dispersing out of the channel. A release within the channel occurs at radius = 0, which travels in the down-slope direction of the channel, T .

Between $r = 0$ and $r = L$, the dispersion width is defined as follows:

$$\begin{aligned} Y &= \sigma_y && \text{when } W > \sigma_y \\ Y &= W = \sigma_y && \text{when } W = \sigma_y \text{ or } W < \sigma_y \end{aligned} \tag{82}$$

where σ_y = lateral dispersion parameter (m).

To simulate the transition in flows at the end of the channel and avoid an abrupt concentration change between the channeled flow and the regional climatological dispersion, a linear interpolation is made between channel and regional concentrations for the direction, T , over the distance, D . This transition distance is assumed to be equal to the channel width, W .

This channeling module is designed to improve the performance of the atmospheric component by accounting for the gross aspects of local channeling in the computation of long-term average exposures. The channeling module provides for directed local plume movement under nocturnal conditions with

9.0 SHORT-TERM AIR CONCENTRATIONS

In addition to the evaluation of potential longer-term chronic impacts, many situations require consideration of potential acute impacts over a shorter time period. The processes are the same as discussed for the long-term impacts; the released material is transported and dispersed by air movement. The difference is the concern for a release occurring over a relatively short time—resulting in a greater range of possible plume concentrations and impacts over a smaller area.

MEPAS computes acute normalized dispersion values applicable to releases of approximately an one hour duration. The standard straight-line, Gaussian model expressed by Equation 45 is used to compute hourly concentrations for a matrix of wind speed, wind direction, and stability conditions. Both statistical and maximum value summaries of the short-term normalized concentrations are provided. For a near-ground-level release, the computed hourly concentrations combined with the frequencies of occurrence for each case (from the climatological joint frequency dispersion summaries) are used to define the 95% and 50% normalized air concentrations at 100 m from the source. For all types of atmospheric releases, the maximum hourly normalized air concentration and its location are provided for each direction. These summaries of short-term air concentrations normalized to a unit release are provided as supplemental information for evaluation of acute exposures.

The roughness influences on dispersion rates and wind speed tend to cancel each other. As a result of surface-induced mechanical mixing, the local surface roughness influences local dispersion rates. All other factors being equal, a site with a smoother surface will appear to have smaller dilution rates than a site with a rougher surface. However the surface roughness will also change the near-surface wind speed; there will be faster near-surface winds over a smooth surface compared to a rough surface. The surface-roughness induced changes in the vertical and horizontal dilution rates tend to be greater than the opposing change in the near-surface wind speeds. The

result is that, all other factors being equal, the estimated acute normalized air concentrations are larger over smooth surfaces than over rough surfaces.

The computed hourly normalized dispersion values are estimates for potential ambient conditions that result in the maximum acute exposures. The Gaussian model applies best to a site located on a uniform flat plane. The model is used only as an approximation for sites located on other types of terrain.

10.0 SUMMARY

The atmospheric pathway component of the MEPAS model provides estimates of potential ambient air concentrations and deposition rates. These outputs of the atmospheric pathway component are input to the MEPAS exposure assessment components. The atmospheric and surface deposition concentrations are computed using standard Gaussian dispersion models that use local climatologic site data. This computation accounts for influences such as the regional patterns of surface roughness and terrain heights. Major removal and decay mechanisms are also incorporated. This deposition computation provides estimates of both regional average and surface-specific contaminant deposition rates. A complex-terrain option accounts for the influence of local nocturnal wind channeling near the source.



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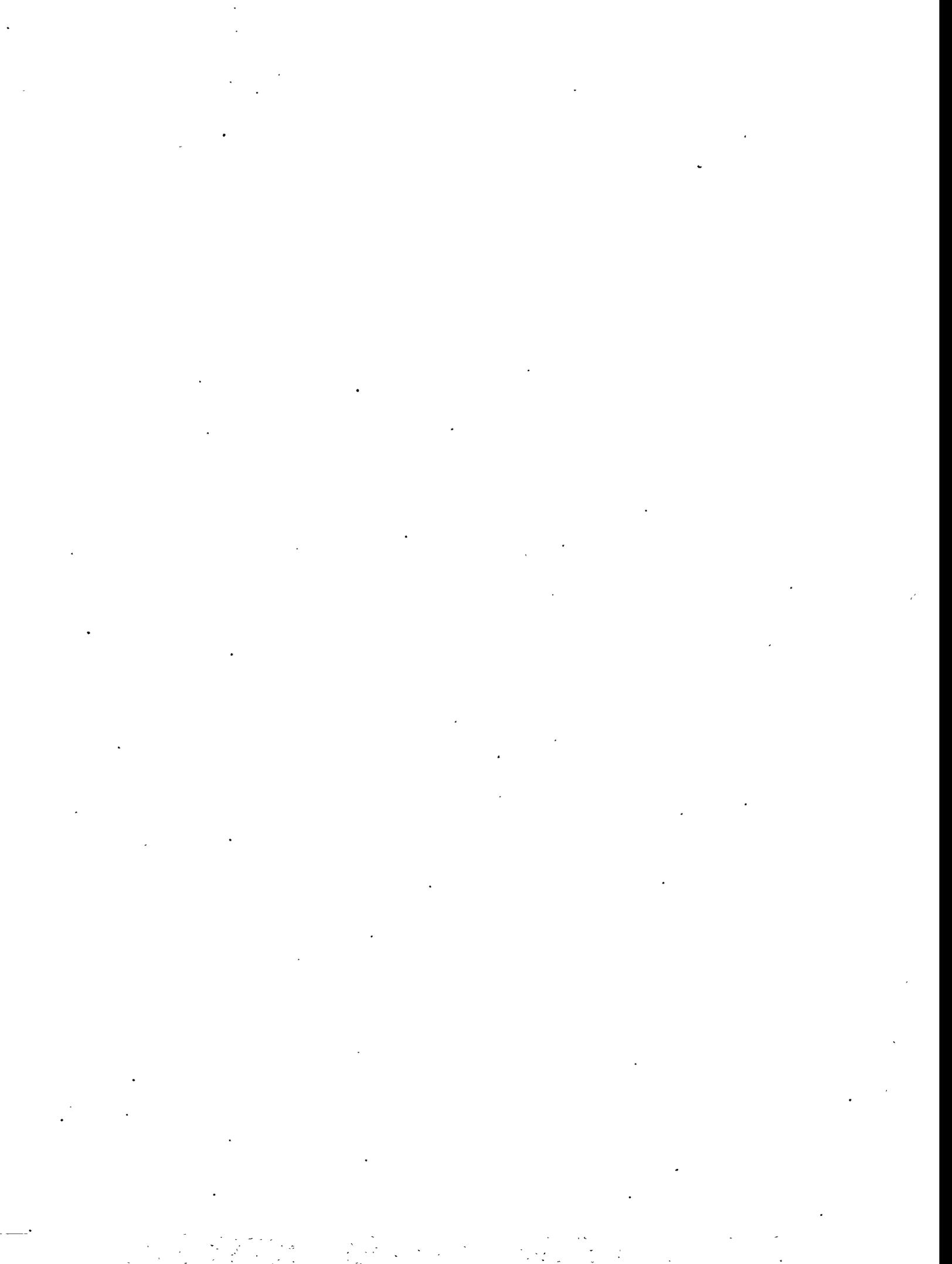
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